

Scientific and Technical Information Center

SEARCH REQUEST FORM 256470

Requester's Full Name: Cecilia Jaisle Examiner #: 43 DE Date: 4-3-78
 At Unit: 1034 Phone Number: 2-9931 Serial Number: 10590786
 Location (City/County): READING (Attala St) Results Format Preferred (check): PAPER DISK

To ensure an efficient and quality search, please attach a copy of the cover sheet, claims, and abstract or file cut the following:

Title of Invention: See Bib Data Sheet

Invention (please provide full text):

Issuing Priority Date:

Assignee:

For a detailed description of the selected patent and its claim(s) go to the assigned module by selecting species or structures, keywords, generation, concepts, and entity numbers, and combine it with the concept or entity of a secondary or third source that may have a special meaning. (See examples or relevant sections, entries, etc., below.)

*For Sequence Searches Only: Please include all protein information (amino acid, chemical, or derived protein sequence) in its initial form appropriate serial number.

See claims attached. Please do structure search and invention name(s) search. Display results to show identification of source, and R.N., compound name & structure of identified compounds. Search compounds of formula I where A is phenyl with addition as noted:

Please call with any questions

STAFF USE ONLY

| | Type of Search | Vendors and cost where applicable |
|-----------------------------|----------------|--|
| Searcher: | NA Request #: | SDA Dialog |
| Searcher Name #: | SI Request #: | Cambridge, Cambridge |
| Searcher Location: | Merge #: | Varies, WWW/Internet |
| First Searcher Merged #: | Offcomple | Academic resource systems |
| Date Completed: | Urgent: | Symantec, Oracle, SISB, SciWorld, SciWorld |
| Searcher Log & Review Form: | Normal: | Informex, SISB, SciWorld, SciWorld |
| Other Info: | None: | |

Author Search

=> FILE HCPLUS
FILE 'HCPLUS' ENTERED AT 12:18:42 ON 15 APR 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 15 Apr 2008 VOL 148 ISS 16
FILE LAST UPDATED: 14 Apr 2008 (20080414/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

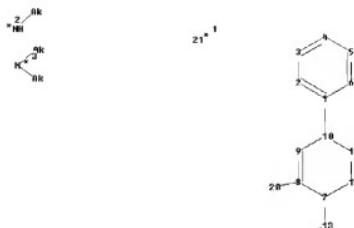
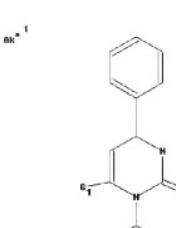
This file contains CAS Registry Numbers for easy and accurate substance identification.

'OBI' IS DEFAULT SEARCH FIELD FOR 'HCPLUS' FILE

=> D QUE L44
L17 17 SEA FILE=HCPLUS ABB=ON PLU=ON GIELEN-HAERTWIG H?/AU
L18 233 SEA FILE=HCPLUS ABB=ON PLU=ON ALBRECHT B?/AU
L19 92 SEA FILE=HCPLUS ABB=ON PLU=ON KELDENICH J?/AU
L20 843 SEA FILE=HCPLUS ABB=ON PLU=ON LI V?/AU
L21 51 SEA FILE=HCPLUS ABB=ON PLU=ON PERNERSTORFER J?/AU
L22 117 SEA FILE=HCPLUS ABB=ON PLU=ON SCHLEMMER K?/AU
L23 22 SEA FILE=HCPLUS ABB=ON PLU=ON TELAN L?/AU
L24 1299 SEA FILE=HCPLUS ABB=ON PLU=ON (L17 OR L18 OR L19 OR L20 OR
 L21 OR L22 OR L23)
L38 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation:
Uploading strD.str



chain nodes :

19 20 21 27 28 29 30 31

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18

chain bonds :

1-10 7-13 8-20 12-19 27-28 29-30 29-31

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18 14-15
15-16 16-17 17-18

exact/norm bonds :

1-10 7-8 7-12 7-13 8-9 8-20 9-10 10-11 11-12 12-19 13-14 13-18 14-15
15-16 16-17 17-18 27-28 29-30 29-31

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

G1:H,NH2,[*1],[*2],[*3]

G2:C,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS
20:CLASS 21:CLASS

27:CLASS 28:Atom 29:CLASS 30:CLASS 31:CLASS

Element Count :

Node 21: Limited

C,C1-4

L40 768 SEA FILE=REGISTRY SSS FUL L38
 L42 20 SEA FILE=HCAPLUS ABB=ON PLU=ON L40
 L43 15 SEA FILE=HCAPLUS ABB=ON PLU=ON L42 AND (PRY<=2005 OR

AY<=2005 OR PY<=2005)
L44 5 SEA FILE=HCAPLUS ABB=ON PLU=ON L24 AND L43

=> FILE WPIX
FILE 'WPIX' ENTERED AT 12:18:52 ON 15 APR 2008
COPYRIGHT (C) 2008 THE THOMSON CORPORATION

FILE LAST UPDATED: 12 APR 2008 <20080412/UP>
MOST RECENT THOMSON SCIENTIFIC UPDATE: 200824 <200824/DW>
DERWENT WORLD PATENTS INDEX SUBSCRIBER FILE, COVERS 1963 TO DATE

>>> IPC Reform backfile reclassification has been loaded to the end of November 2007. No update date (UP) has been created for the reclassified documents, but they can be identified by 20060101/UPIC and 20061231/UPIC, 20070601/UPIC, 20071001/UPIC and 20071130/UPIC. <<<

FOR A COPY OF THE DERWENT WORLD PATENTS INDEX STN USER GUIDE,
PLEASE VISIT:

http://www.stn-international.de/training_center/patents/stn_guide.pdf

FOR DETAILS OF THE PATENTS COVERED IN CURRENT UPDATES, SEE
<http://scientific.thomson.com/support/patents/coverage/latestupdates/>

EXPLORE DERWENT WORLD PATENTS INDEX IN STN ANAVIST, VERSION 2.0:

http://www.stn-international.com/archive/presentations/DWPPIAnaVist2_0710.pdf

>>> XML document distribution format now available - See HELP XMDOC <<<

>>> ECLA Codes and Current US National Classifications have been added -
see NEWS and HELP CHANGE <<<

>>> HELP for European Patent Classifications see HELP ECLA, HELP ICO <<<

>>> Updated PDF files in the following links:

http://www.stn-international.de/stndatabases/details/ico_0803.zip

http://www.stn-international.de/stndatabases/details/epc_0803.zip

Supplement of all changed ECLA items:

[>>> http://www.stn-international.de/stndatabases/details/ecla_0803s.zip](http://www.stn-international.de/stndatabases/details/ecla_0803s.zip)

'BI,ABEX' IS DEFAULT SEARCH FIELD FOR 'WPIX' FILE

=> D QUE L48
L17 17 SEA FILE=HCAPLUS ABB=ON PLU=ON GIELEN-HAERTWIG H?/AU
L18 233 SEA FILE=HCAPLUS ABB=ON PLU=ON ALBRECHT B?/AU
L19 92 SEA FILE=HCAPLUS ABB=ON PLU=ON KELDENICH J?/AU
L20 843 SEA FILE=HCAPLUS ABB=ON PLU=ON LI V?/AU
L21 51 SEA FILE=HCAPLUS ABB=ON PLU=ON PERNERSTORFER J?/AU
L22 117 SEA FILE=HCAPLUS ABB=ON PLU=ON SCHLEMMER K?/AU
L23 22 SEA FILE=HCAPLUS ABB=ON PLU=ON TELAN L?/AU
L24 1299 SEA FILE=HCAPLUS ABB=ON PLU=ON (L17 OR L18 OR L19 OR L20 OR
L21 OR L22 OR L23)
L38 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

L46 117 SEA FILE=WPIX SSS FUL L38
L47 7 SEA FILE=WPIX ABB=ON PLU=ON L46/DCR
L48 5 SEA FILE=WPIX ABB=ON PLU=ON L47 AND L24

=> DUP REM L44 L48
FILE 'HCAPLUS' ENTERED AT 12:19:02 ON 15 APR 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)

FILE 'WPIX' ENTERED AT 12:19:02 ON 15 APR 2008
COPYRIGHT (C) 2008 THE THOMSON CORPORATION
PROCESSING COMPLETED FOR L44
PROCESSING COMPLETED FOR L48
L54 6 DUP REM L44 L48 (4 DUPLICATES REMOVED)
ANSWERS '1-5' FROM FILE HCAPLUS
ANSWER '6' FROM FILE WPIX

=> D IBIB ED ABS FHITSTR L54 1-5; D IBIB AB HITSTR 6 L54

L54 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 1
ACCESSION NUMBER: 2006:1608538 HCAPLUS Full-text
DOCUMENT NUMBER: 145:58204
TITLE: Crystal structure of human neutrophil elastase and
uses in drug discovery
INVENTOR(S): Reinemer, Peter; Giesen-Haertwig, Heike;
Rosentreter, Ulrich; Li, Voikhart; Harrenga,
Axel; Schomburg, Dietmar; Niefeld, Karsten; Hansen,
Guido
PATENT ASSIGNEE(S): Bayer Healthcare AG, Germany
SOURCE: PCT Int. Appl., 123 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|----------------|
| WO 2006063792 | A2 | 20060622 | WO 2005-EP13370 | 20051213 <-- |
| WO 2006063792 | A3 | 20070412 | | |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GO, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA | | | | |
| CA 2590851 | A1 | 20060622 | CA 2005-2590851 | 20051213 <-- |
| EP 1828233 | A2 | 20070905 | EP 2005-819949 | 20051213 <-- |
| R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, MK, YU | | | | |
| PRIORITY APPLN. INFO.: | | | EP 2004-29768 | A 20041216 <-- |
| | | | WO 2005-EP13370 | W 20051213 <-- |

ED Entered STN: 23 Jun 2006

AB This invention relates to crystallized human neutrophil elastase and the use of its three-dimensional structure to design modulators for human neutrophil elastase. The crystal structure and the atomic structural coordinates of human neutrophil elastase and inhibitor complexes is disclosed.

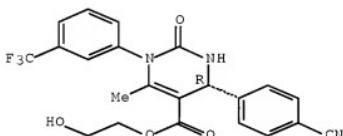
IT 675103-34-1DP, complexes with elastase

RL: BPN (Biosynthetic preparation); BSU (Biological study, unclassified); BUU (Biological use, unclassified); PRP (Properties); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of elastase inhibitor; crystal structure of human neutrophil elastase and uses in drug discovery)

RN 675103-1 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-hydroxyethyl ester, (4R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



L54 ANSWER 2 OF 6 HCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 2

ACCESSION NUMBER: 2005:979623 HCAPLUS [Full-text](#)

DOCUMENT NUMBER: 143:286441

TITLE: Preparation of diaryl-dihydropyrimidin-2-ones as human neutrophil elastase inhibitors

INVENTOR(S): Gielen-Haertwig, Heike; Albrecht, Barbara; Keldenich, Joerg; Li, Volkhardt; Pernerstorfer, Josef; Schiemmer, Karl-Heinz; Teian, Leila

PATENT ASSIGNEE(S): Bayer Healthcare A.-G., Germany

SOURCE: PCT Int. Appl., 141 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|--------------|
| WO 2005082864 | A1 | 20050909 | WO 2005-EP1486 | 20050215 <-- |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, | | | | |

RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,
MR, NE, SN, TD, TG
 CA 2557271 A1 20050909 CA 2005-2557271 20050215 <--
 EP 1723121 A1 20061122 EP 2005-707386 20050215 <--
 R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
 IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR
 JP 2007524696 T 20070830 JP 2007-500099 20050215 <--
 US 20080064704 A1 20080313 US 2007-590770 20070618 <--
 PRIORITY APPLN. INFO.: EP 2004-4314 A 20040226 <--
 WO 2005-EP1486 W 20050215 <--

OTHER SOURCE(S): MARPAT 143:286441

ED Entered STN: 08 Sep 2005

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

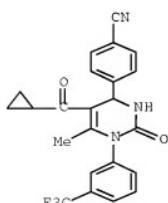
AB Title compds. I [A = aryl or heteroaryl ring; R1, R2 and R3 independently = H, halo, nitro, etc.; R4 = (un)substituted alkyl, cycloalkylcarbonyl, alkylcarbonyl, etc.; R5 = (un)substituted alkyl; R6 = H, formyl, aminocarbonyl, etc.; R7 = cyano, OH, nitro, etc.; V, W, X, Y and Z independently = CH or N wherein the ring contains either 0, 1 or 2 nitrogen atoms] and their pharmaceutically acceptable salts, are prepared and disclosed as human neutrophil elastase (HNE) inhibitors. Thus, e.g., II was prepared by cyclization of N-[3-(trifluoromethyl)phenyl]urea and 4-cyanobenzaldehyde with ethyl-3-oxobutanoate and subsequent reduction using LAH. The activity of I against HNE was evaluated in an in vitro enzyme assay utilizing a fluorogenic peptide substrate and it was revealed that selected compds. of the invention possessed IC50 values in the range of 5 up to 1000 nM. I as inhibitors of human neutrophil elastase should prove useful in the treatment of chronic obstructive pulmonary diseases, acute coronary syndrome, acute myocardial infarction and heart failure development. Pharmaceutical compns. comprising I are disclosed.

IT 864250-62-4P

RL: PAC (Pharmacological activity); PEP (Physical, engineering or chemical process); PYP (Physical process); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); RACT (Reactant or reagent); USES (Uses) (preparation of diaryl-dihydropyrimidin-2-ones as human neutrophil elastase inhibitors)

RN 864250-62-4 HCPLUS

CN Benzonitrile, 4-[5-(cyclopropylcarbonyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-4-pyrimidinyl] (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

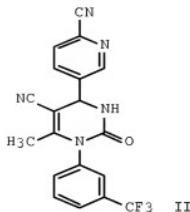
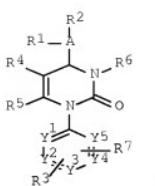
L54 ANSWER 3 OF 6 HCPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 3
 ACCESSION NUMBER: 2005:979622 HCPLUS Full-text
 DOCUMENT NUMBER: 143:286440
 TITLE: Preparation of tetrasubstituted pyrimidin-2-ones as
 human neutrophil elastase inhibitors
 INVENTOR(S): Gielen-Haertwig, Heike; Albrecht,
 Barbara; Keldenich, Joerg; Li,
 Volkhart; Pernerstorfer, Josef;
 Schlemmer, Karl-Heinz; Telan, Leila
 PATENT ASSIGNEE(S): Bayer Healthcare A.-G., Germany
 SOURCE: PCT Int. Appl., 119 pp.
 CODEN: PIXDZ2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|--|------|----------|-----------------|----------------|
| WO 2005082863 | A2 | 20050909 | WO 2005-EP1487 | 20050215 <-- |
| WO 2005082863 | A3 | 20051222 | | |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| CA 2557272 | A1 | 20050909 | CA 2005-2557272 | 20050215 <-- |
| EP 1730121 | A2 | 20061213 | EP 2005-707387 | 20050215 <-- |
| R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR | | | | |
| JP 2007523931 | T | 20070823 | JP 2007-500100 | 20050215 <-- |
| US 20080021053 | A1 | 20080124 | US 2007-590786 | 20070720 <-- |
| PRIORITY APPLN. INFO.: | | | EP 2004-4315 | A 20040226 <-- |
| | | | WO 2005-EP1487 | W 20050215 <-- |

OTHER SOURCE(S): MARPAT 143:286440

ED Entered STN: 08 Sep 2005

GI



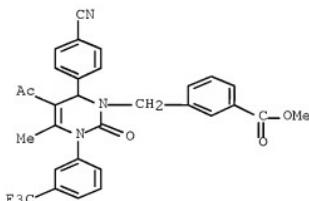
AB Title compds. I [A = heteroaryl ring; R1-3 = H, halo, NO₂, etc.; R4 = CF₃CO, alkylcarbonyl, etc.; R5 = alkyl, alkoxy, etc.; R6 = T-U; T = alkanediyl, akenediyl; U = aryl, heteroaryl, etc.; R7 = halo, NO₂, CN, etc.; Y1-5 = independently CH, N wherein the ring contains 0-2 N atoms] and analogs are prepared. For instance, II is prepared in 6 steps from 2-bromo-5-methylpyridine, allyl 3-oxobutanoate and N-[3-(trifluoromethyl)phenyl]urea. II has an IC₅₀ = 70 nM for human neutrophil elastase (HNE). I are useful for the treatment of chronic obstructive pulmonary diseases, acute coronary syndrome, acute myocardial infarction and heart failure development.

IT 864150-42-5P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of tetrasubstituted pyrimdin-2-ones as human neutrophil elastase inhibitors)

RN 864150-42-5 HCPLUS

CN Benzoic acid, 3-[(5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl)methyl]-, methyl ester (CA INDEX NAME)



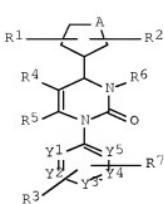
INVENTOR(S): Gielen, Heike; Li, Volkart; Rosentreter, Ulrich; Schlemmer, Karl-heinz;
 Allerheiligen, Swen; Tsian, Leila;
 Baerfacker, Lars; Keidenich, Joerg;
 Fitzgerald, Mary F.; Nash, Kevin; Albrecht,
 Barbara; Meurer, Dirk
 PATENT ASSIGNEE(S): Bayer Healthcare Ag, Germany
 SOURCE: PCT Int. Appl., 121 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|----------------|
| WO 2004024700 | A1 | 20040325 | WO 2003-EP9525 | 20030828 <-- |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| GB 2392910 | A | 20040317 | GB 2003-15870 | 20030707 <-- |
| CA 2498051 | A1 | 20040325 | CA 2003-2498051 | 20030828 <-- |
| AU 2003282006 | A1 | 20040430 | AU 2003-282006 | 20030828 <-- |
| EP 1546113 | A1 | 20050629 | EP 2003-773613 | 20030828 <-- |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK | | | | |
| BR 2003014186 | A | 20050809 | BR 2003-14186 | 20030828 <-- |
| JP 2006507355 | T | 20060302 | JP 2004-571738 | 20030828 <-- |
| NZ 538670 | A | 20070126 | NZ 2003-538670 | 20030828 <-- |
| MX 2005PA02644 | A | 20050920 | MX 2005-PA2644 | 20050309 <-- |
| NO 2005001726 | A | 20050407 | NO 2005-1726 | 20050407 <-- |
| US 20060160801 | A1 | 20060720 | US 2005-527391 | 20051021 <-- |
| PRIORITY APPLN. INFO.: | | | | |
| | | | GB 2002-20962 | A 20020910 <-- |
| | | | GB 2002-26609 | A 20021114 <-- |
| | | | GB 2003-15870 | A 20030707 <-- |
| | | | WO 2003-EP9525 | W 20030828 <-- |

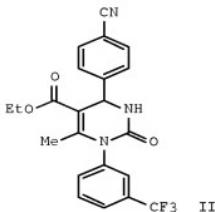
OTHER SOURCE(S): MARPAT 140:287406

ED Entered STN: 28 Mar 2004

GI



I

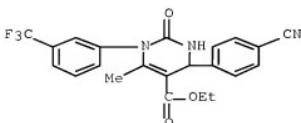


AB Title compds. I [wherein A = hetero/aryl; R1, R2, R3 = independently H, halo, NO₂, CN, OH and derivs., (un)substituted alkyl, R4 = CN, trifluoromethylcarbonyl, alkenoxycarbonyl, hydroxycarbonyl, aryl/alkylaminocarbonyl, (un)substituted heteroarylcarbonyl, heterocyclcarbonyl, heteroaryl, heterocycl, alkylcarbonyl, alkoxy carbonyl, mono- and dialkylaminocarbonyl; R5 = NH₂, (un)substituted alkyl; R6 = H, formyl, N-(alkylsulfonyl)-N-(alkylsulfonyl)-N- (alkyl)/aminocarbonyl, heteroarylcarbonyl, heterocyclcarbonyl, cycloalkylcarbonyl, (un)substituted alkyl, mono- and dialkylaminocarbonyl, alkylcarbonyl, alkoxy carbonyl, heteroaryl, heterocycl, etc.; R7 = halo, NO₂, CN, OH, (un)substituted alkyl, alkoxy; Y1, Y2, Y3, Y4, Y5 = independently CH or N; and their salts, hydrates, and/or solvates, and their tautomeric forms] were prepared as human neutrophil elastase (HNE) inhibitors. For example, II was prepared, in 91% yield, by cyclocondensation of N-[3-(trifluoromethyl)phenyl]urea with 4-cyanobenzaldehyde and Et 3-oxobutanoate. In an in vitro assay, II displayed an IC₅₀ value of 8 nM for HNE inhibition. Thus, I are useful for treatment of acute and chronic inflammation, ischemic and remodelling processes, in particular chronic obstructive pulmonary diseases.

IT 671775-85-2R, Ethyl 4-(4-cyanophenyl)-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-1,2,3,4-tetrahydro-5-pyrimidinecarboxylate
RL: PAC (Pharmacological activity); PEP (Physical, engineering or chemical process); PYP (Physical process); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); RACT (Reactant or reagent); USES (Uses)
 (human neutrophil elastase inhibitor; preparation of pyrimidinones as human neutrophil elastase inhibitors)

RN 671775-85-2 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



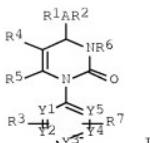
L54 ANSWER 5 OF 6 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2004:213317 HCAPLUS Full-text
 DOCUMENT NUMBER: 140:253573
 TITLE: Preparation of 2-oxopyrimidines as human leukocyte
 elastase (HNE) inhibitors
 INVENTOR(S): Gielen, Heike; Li, Volkhart Min-jian;
 Rosentreter, Ulrich; Schiemmer, Karl-heinz;
 Allerheiligen, Swen; Teian, Leila;
 Baerfacker, Lars; Keldenich, Joerg;
 Albrecht, Barbara; Meurer, Dirk; Fitzgerald,
 Mary; Nash, Kevin
 PATENT ASSIGNEE(S): Bayer Ag, Germany
 SOURCE: Brit. UK Pat. Appl., 117 pp.
 CODEN: BAXXDU
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|--|------|----------------|-----------------|--------------|
| GB 2392910 | A | 20040317 | GB 2003-15870 | 20030707 <-- |
| CA 2498051 | A1 | 20040325 | CA 2003-2498051 | 20030828 <-- |
| WO 2004024700 | A1 | 20040325 | WO 2003-EP9525 | 20030828 <-- |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KE, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| AU 2003282006 | A1 | 20040430 | AU 2003-282006 | 20030828 <-- |
| EP 1546113 | A1 | 20050629 | EP 2003-773613 | 20030828 <-- |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK | | | | |
| BR 2003014186 | A | 20050809 | BR 2003-14186 | 20030828 <-- |
| CN 1732159 | A | 20060208 | CN 2003-824983 | 20030828 <-- |
| JP 2006507355 | T | 20060302 | JP 2004-571738 | 20030828 <-- |
| NZ 538670 | A | 20070126 | NZ 2003-538670 | 20030828 <-- |
| ZA 2005001964 | A | 20060531 | ZA 2005-1964 | 20050308 <-- |
| MX 2005PA02644 | A | 20050920 | MX 2005-PA2644 | 20050309 <-- |
| NO 2005001726 | A | 20050407 | NO 2005-1726 | 20050407 <-- |
| US 20060160801 | A1 | 20060720 | US 2005-527391 | 20051021 <-- |
| PRIORITY APPLN. INFO.: | | | | |
| | | GB 2002-20962 | A | 20020910 <-- |
| | | GB 2002-26609 | A | 20021114 <-- |
| | | GB 2003-15870 | A | 20030707 <-- |
| | | WO 2003-EP9525 | W | 20030828 <-- |

OTHER SOURCE(S): MARPAT 140:253573

ED Entered STN: 17 Mar 2004

GI



AB Title compds. (I; A = aryl, heteroaryl; R1-R3 = H, OH, halo, NO₂, cyano, (substituted) alkyl, alkoxy; R4 = F₃CCO, (substituted) alkylcarbonyl, alkoxycarbonyl, alkenyloxycarbonyl, CO₂H, arylcarbonyl, heteroaryl, heterocyclyl, cyano, etc.; R5 = (substituted) alkyl, amino; R6 = H, CHO, CONH₂, (substituted) alkyl, alkoxy carbonyl, alkylsulfonylaminocarbonyl, heteroaryl, heterocyclyl, etc.; R7 = halo, NO₂, cyano, OH, (substituted) alkyl, alkoxy; Y1-Y5 = CH, N, wherein the ring contains 0-2 NJ, were prepared Thus, 3-trifluoromethylphenylurea, 4-cyanobenzaldehyde, Et 3-oxobutyrate, and polyphosphoric acid Et ester were refluxed 18 h in THF to give 91% Et 4-(4-cyanophenyl)-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-1,2,3,4-tetrahydro-5-pyrimidinecarboxylate. The latter inhibited HNE with IC₅₀ = 8 nM.

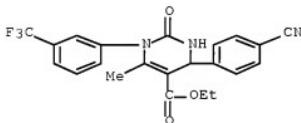
IT 671775-85-2F

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of 2-oxopyrimidines as human leukocyte elastase inhibitors)

RN 671775-85-2 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L54 ANSWER 6 OF 6 WPIX COPYRIGHT 2008 THE THOMSON CORP on STN
 ACCESSION NUMBER: 2008-B43885 [10] WPIX
 DOC. NO. CPI: C2008-040102 [10]
 TITLE: Use of 1,4-diaryl-dihydropyrimidin-2-one derivative for producing a medicament for the treatment and/or prophylaxis of e.g. pulmonary arterial hypertension, chronic-obstructive lung diseases and sleep apnea syndrome

DERWENT CLASS: B03
 INVENTOR: GIELEN-HAERTWIG B; KLEIN M; LI V;
 LI V M; LUSTIG K; MEIBOM D; NUSSBAUM F; SANDNER
 P; SCHAEFER S; VON NUSSBAUM F
 PATENT ASSIGNEE: (FARB-C) BAYER HEALTHCARE AG
 COUNTRY COUNT: 120

PATENT INFO ABBR.:

| PATENT NO | KIND | DATE | WEEK | LA | PG | MAIN IPC |
|--------------------|----------|-----------|----------|-------|----|----------|
| DE 102006031314 A1 | 20080103 | (200810)* | DE | 34[0] | | |
| WO 2008003412 | A1 | 20080110 | (200810) | DE | | |

APPLICATION DETAILS:

| PATENT NO | KIND | APPLICATION | DATE |
|--------------------|------|----------------------|----------|
| DE 102006031314 A1 | | DE 2006-102006031314 | 20060701 |
| WO 2008003412 A1 | | WO 2007-EP5579 | 20070625 |

PRIORITY APPLN. INFO: DE 2006-102006031314 20060701

AB DE 102006031314 A1 UPAB: 20080208

NOVELTY - Use of 1,4-diaryl-dihydropyrimidin-2-one derivative (I) or its salts, solvates or solvates of the salts, for producing a medicament for the treatment and/or prophylaxis of pulmonary arterial hypertension.

DETAILED DESCRIPTION - Use of 1,4-diaryl-dihydropyrimidin-2-one derivative of formula (I) or its salts, solvates or solvates of the salts, for producing a medicament for the treatment and/or prophylaxis of the pulmonary arterial hypertension.

R1 = H, -(CH₂)nC(=O)-O-R5 or benzoic acid of formula (a) or (b);

R5 = H or 1-4C-alkyl;

R2 = CN or -C(=O)-R6 or -C(=O)-O-R6;

R6 = 1-6C-alkyl or 3-6C-cycloalkyl (which is partially or substituted two times with hydroxy, 1-4C-alkoxy, hydroxycarbonyl, amino, mono- and/or di-1-4C-alkylamino, where respectively, CH₂ is replaced with an O-atom);

R3, R4 = H, F or Cl;

X = CH or N; and

asterisk = connecting place with the N-atom.

INDEPENDENT CLAIMS are included for:

(1) a combination comprising (I) and an active substance from kinase-inhibitor, stimulator and activator of the soluble guanylate cyclase, prostacyclin-analogues, endothelium receptor-antagonist and phosphodiesterase-inhibitors;

(2) a medicament comprising the combination; and

(3) method for the treatment and/or prophylaxis of the pulmonary arterial hypertension with humans and animals by administering (I), the combination or the medicament in combination with inert, non-toxic auxiliary materials.

ACTIVITY - Hypotensive; Respiratory-Gen; Vulnerary; Respiratory-gen.; CNS-Gen; Thrombolytic; Antiinflammatory.

MECHANISM OF ACTION - Neutrophile elastase inhibitor. The neutrophile elastase inhibitory activity of (I) was tested using human neutrophile elastase. The result showed that (I) exhibited a median inhibitory concentration (IC50) of 14.8 nM.

USE - (I) is useful as medicament for the treatment and/or prophylaxis of the pulmonary arterial hypertension with left arterial or left ventricle diseases, left-sided valvular defect, chronic-obstructive lung diseases, interstitial lung diseases, sleep apnea syndrome, diseases with alveolar hypoventilation, Acosta's disease, development of pulmonary disorders, chronic

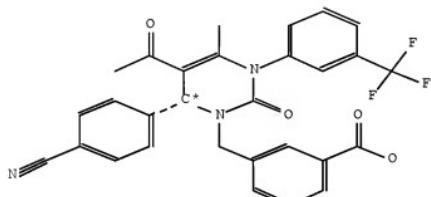
thrombotic and/or embolic diseases, together with sarcoidosis, histiocytosis X or lymphangiomyomatosis, pulmonary arterial hypertension, which is caused from outside by vascular compression (claimed).

ADVANTAGE - (I) is low-molecular, non-reactive, selective and potent inhibitors of neutrophile elastase and shows high bioavailability after oral administration and/or good solubility for the parenteral application.

AN.S DCR-1556396

CN.S 3-[(R)-5-Acetyl-6-(4-cyano-phenyl)-4-methyl-2-oxo-3-(3-trifluoromethyl-phenyl)-3,6-dihydro-2H-pyrimidin-1-ylmethyl]-benzoic acid

SDCN RAS1SU



AN.S DCR-1332800

CN.S (R)-4-(4-Cyano-phenyl)-6-methyl-2-oxo-1-(3-trifluoromethyl-phenyl)-1,2,3,4-tetrahydro-pyrimidine-5-carboxylic acid 2-hydroxy-ethyl ester

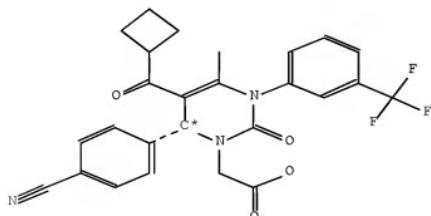
SDCN RANA4W

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AN.S DCR-1556397

CN.S [(R)-6-(4-Cyano-phenyl)-5-cyclobutanecarbonyl-4-methyl-2-oxo-3-(3-trifluoromethyl-phenyl)-3,6-dihydro-2H-pyrimidin-1-yl]-acetic acid

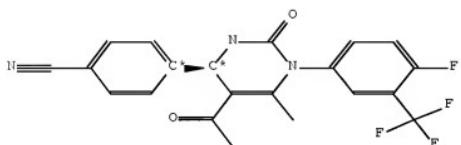
SDCN RAS1SV



AN.S DCR-1556399

CN.S 4-[(R)-5-Acetyl-1-(4-fluoro-3-trifluoromethyl-phenyl)-6-methyl-2-oxo-
1,2,3,4-tetrahydro-pyrimidin-4-yl]-benzonitrile

SDCN RAS1SX



Structure Search

```
=> FILE HCAPLUS
FILE 'HCAPLUS' ENTERED AT 12:19:55 ON 15 APR 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)
```

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 15 Apr 2008 VOL 148 ISS 16
FILE LAST UPDATED: 14 Apr 2008 (20080414/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.
'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

```
=> D QUE L43
L38          STR
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *
```

Structure attributes must be viewed using STN Express query preparation.
L40 768 SEA FILE=REGISTRY SSS FUL L38
L42 20 SEA FILE=HCAPLUS ABB=ON PLU=ON L40
L43 15 SEA FILE=HCAPLUS ABB=ON PLU=ON L42 AND (PRY<=2005 OR
AY<=2005 OR PY<=2005)

```
=> S L43 NOT L44
L55      10 L43 NOT L44
```

```
=> FILE WPIX
FILE 'WPIX' ENTERED AT 12:20:16 ON 15 APR 2008
COPYRIGHT (C) 2008 THE THOMSON CORPORATION
```

FILE LAST UPDATED: 12 APR 2008 <20080412/UP>
MOST RECENT THOMSON SCIENTIFIC UPDATE: 200824 <200824/DW>
DERWENT WORLD PATENTS INDEX SUBSCRIBER FILE, COVERS 1963 TO DATE

```
>>> IPC Reform backfile reclassification has been loaded to the end of
November 2007. No update date (UP) has been created for the
reclassified documents, but they can be identified by
20060101/UPIC and 20061231/UPIC, 20070601/UPIC, 20071001/UPIC and
20071130/UPIC. <<
```

FOR A COPY OF THE DERWENT WORLD PATENTS INDEX STN USER GUIDE,
PLEASE VISIT:

http://www.stn-international.de/training_center/patents/stn_guide.pdf

FOR DETAILS OF THE PATENTS COVERED IN CURRENT UPDATES, SEE
<http://scientific.thomson.com/support/patents/coverage/latestupdates/>

EXPLORE DERWENT WORLD PATENTS INDEX IN STN ANAVIST, VERSION 2.0:

http://www.stn-international.com/archive/presentations/DWPPIAnaVist2_0710.pdf

>>> XML document distribution format now available - See HELP XMLDOC <<<

>>> ECLA Codes and Current US National Classifications have been added -
see NEWS and HELP CHANGE <<<

>>> HELP for European Patent Classifications see HELP ECLA, HELP ICO <<<

>>> Updated PDF files in the following links:

http://www.stn-international.de/stndatabases/details/ico_0803.zip

http://www.stn-international.de/stndatabases/details/epc_0803.zip

Supplement of all changed ECLA items:

http://www.stn-international.de/stndatabases/details/ecla_0803s.zip <<<

'BI,ABEX' IS DEFAULT SEARCH FIELD FOR 'WPIX' FILE

=> D QUE L47

L38 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

L46 117 SEA FILE=WPIX SSS FUL L38

L47 7 SEA FILE=WPIX ABB=ON PLU=ON L46/DCR

=> S L47 NOT L48

L56 2 L47 NOT L48

=> FILE BEILSTEIN

FILE 'BEILSTEIN' ENTERED AT 12:20:36 ON 15 APR 2008

COPYRIGHT (c) 2008 Beilstein-Institut zur Foerderung der Chemischen Wissenschaften
licensed to Beilstein GmbH and MDL Information Systems GmbH

FILE LAST UPDATED ON April 1, 2008

FILE COVERS 1771 TO 2008.

*** FILE CONTAINS 10,322,808 SUBSTANCES ***

>>> PLEASE NOTE: Reaction Data and substance data are stored in
separate documents and can not be searched together in one query.
Reaction data for BEILSTEIN compounds may be displayed
immediately with the display codes PRE (preparations) and REA
(reactions). A substance answer set retrieved after the search
for a chemical name, a compounds with available reaction
information by combining with PRE/FA, REA/FA or more generally
with RX/FA. The BEILSTEIN Registry Number (BRN) is the link
between a BEILSTEIN compound and belonging reactions. For mo
detailed reaction searches BRNs can be searched as reaction
partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

* PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST. *
* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE *
* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE *
* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS. *
* FOR PRICE INFORMATION SEE HELP COST *

>>> Price change as of January 1st, 2008: Connect Time and Structure
Search fees re-introduced. See NEWS and HELP COST <<<

=> D QUE L53
L38 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L50 23 SEA FILE=BEILSTEIN SSS FUL L38
L51 20 SEA FILE=BEILSTEIN ABB=ON PLU=ON L50 AND BABSAN/FA
L53 3 SEA FILE=BEILSTEIN ABB=ON PLU=ON L50 NOT L51

=> FILE BABS
FILE 'BABS' ENTERED AT 12:20:45 ON 15 APR 2008
COPYRIGHT (c) 2008 Beilstein-Institut zur Foerderung der Chemischen Wissenschaften
licensed to Beilstein GmbH and MDL Information Systems GmbH

FILE LAST UPDATED: 17 MAR 2008 <20080317/UP>
FILE COVERS 1980 TO DATE.

=> D QUE L52
L52 6 SEA FILE=BABS ABB=ON PLU=ON (6615225/BABSAN OR 6322274/BABSAN
OR 6679519/BABSAN OR 5898555/BABSAN OR 5545785/BABSAN OR
6058956/BABSAN)

=> DUP REM L55 L56 L53 L52
DUPLICATE IS NOT AVAILABLE IN 'BEILSTEIN'.
ANSWERS FROM THESE FILES WILL BE CONSIDERED UNIQUE
FILE 'HCAPLUS' ENTERED AT 12:21:04 ON 15 APR 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)

FILE 'WPIX' ENTERED AT 12:21:04 ON 15 APR 2008
COPYRIGHT (C) 2008 THE THOMSON CORPORATION

FILE 'BEILSTEIN' ENTERED AT 12:21:04 ON 15 APR 2008
COPYRIGHT (c) 2008 Beilstein-Institut zur Foerderung der Chemischen Wissenschaften
licensed to Beilstein GmbH and MDL Information Systems GmbH

FILE 'BABS' ENTERED AT 12:21:04 ON 15 APR 2008
COPYRIGHT (c) 2008 Beilstein-Institut zur Foerderung der Chemischen Wissenschaften
licensed to Beilstein GmbH and MDL Information Systems GmbH
PROCESSING COMPLETED FOR L55
PROCESSING COMPLETED FOR L56
PROCESSING COMPLETED FOR L53
PROCESSING COMPLETED FOR L52
L57 15 DUP REM L55 L56 L53 L52 (6 DUPLICATES REMOVED)
ANSWERS '1-10' FROM FILE HCAPLUS
ANSWERS '11-13' FROM FILE BEILSTEIN

ANSWERS '14-15' FROM FILE BABs

=> D IBIB ED ABS HITSTR L57 1-10; D IDE ALLREF 11-13 L57; D ALL 14-15 L57

L57 ANSWER 1 OF 15 HCPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 1
 ACCESSION NUMBER: 20061356757 HCPLUS Full-text
 DOCUMENT NUMBER: 146:100714
 TITLE: Preparation of dihydropyrimidone multimers as human neutrophil elastase inhibitors
 INVENTOR(S): Finch, Harry; Edwards, Christine; Ray, Nicholas Charles; Fitzgerald, Mary Frances
 PATENT ASSIGNEE(S): Argenta Discovery Ltd., UK
 SOURCE: PCT Int. Appl., 59pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|--|----------|-----------------|----------------|
| WO 2006136857 | A1 | 20061228 | WO 2006-GB2337 | 20060626 <-- |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HN, HR, HU, ID, IL, IN, IS, JE, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW | RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | |
| EP 1893584 | A1 | 20080305 | EP 2006-755623 | 20060626 <-- |
| R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR | | | | |
| PRIORITY APPLN. INFO.: | | | GB 2005-12940 | A 20050624 <-- |
| | | | WO 2006-GB2337 | W 20060626 |

OTHER SOURCE(S): MARPAT 146:100714

ED Entered STN: 29 Dec 2006

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. represented by the formula M-L-M, wherein L is a linker and each M is independently a group of formula I [A = (hetero)aryl; D = O or S; R1-R3 = independently H, halo, nitro, etc.; R4 = OH, alkyl(carbonyl), amino, etc.; Y1-Y5 = independently C or N, with the proviso that the ring in which they are comprised contains no more than 2 N atoms; R5 = (un)substituted alkyl, -O-alkyl-O-alkyl or amino; R6 = halo, nitro, cyano, etc.; and pharmaceutically acceptable salts, solvates or N-oxides thereof], were prepared as human neutrophil elastase (HNE) inhibitors. For example, II was provided in a multi-step synthesis starting from the reaction of 3-(trifluoromethyl)phenylurea with 4-cyanobenzaldehyde. I were tested for inhibitory activity towards HNE with IC50 values of 1-1000 nM. Thus, I and

their pharmaceutical compns. are useful as human neutrophil elastase inhibitors for the treatment of respiratory diseases (no data).

IT 917813-88-9P 917813-99-2P 917813-97-9P
 917813-98-0P 917813-99-1P 917814-01-6P
 917814-02-9P 917814-13-2P 917814-15-4P
 917814-17-6P

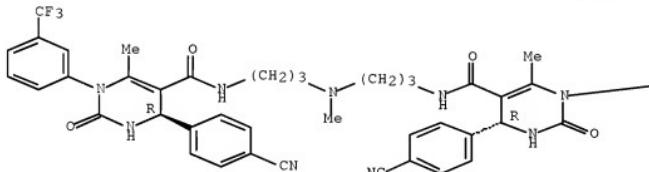
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
 (preparation of dihydropyrimidone multimers as human neutrophil elastase inhibitors)

RN 917813-88-8 HCPLUS

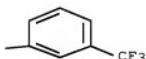
CN 5-Pyrimidinecarboxamide, N,N'-(methylimino)di-3,1-propanediyl]bis[4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, (4R,4'R)- (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

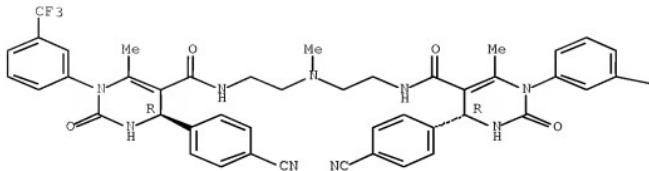


RN 917813-90-2 HCPLUS

CN 5-Pyrimidinecarboxamide, N,N'-(methylimino)di-2,1-ethanediyl]bis[4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, (4R,4'R)- (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

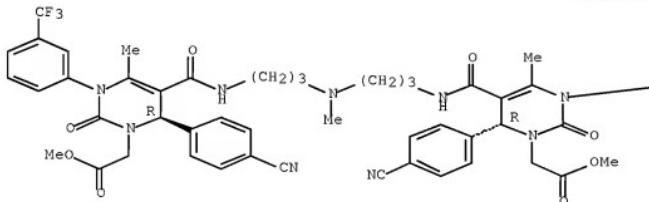
 ---CF_3

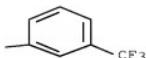
RN 917813-97-9 HCPLUS

CN 1(2H)-Pyrimidineacetic acid, 5,5'-[{methylimino}bis(3,1-propanediyliminocarbonyl)]bis[6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1,1'-dimethyl ester, (6R,6'R)- (CA INDEX NAME)

Absolute stereochemistry.

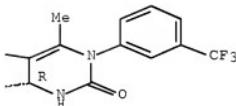
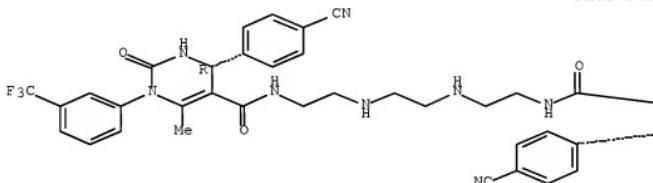
PAGE 1-A





RN 917813-98-0 HCPLUS
 CN 5-Pyrimidinecarboxamide, N,N'-(1,2-ethanediylbis(imino-2,1-ethanediyl))bis[4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, (4R,4'R)- (CA INDEX NAME)

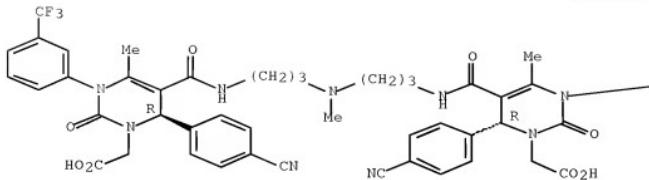
Absolute stereochemistry.



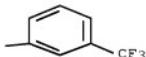
RN 917813-99-1 HCPLUS
 CN 1(2H)-Pyrimidineacetic acid, 5,5'-[{methylimino}bis(3,1-propanediylimino]bis[6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, (6R,6'R)- (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

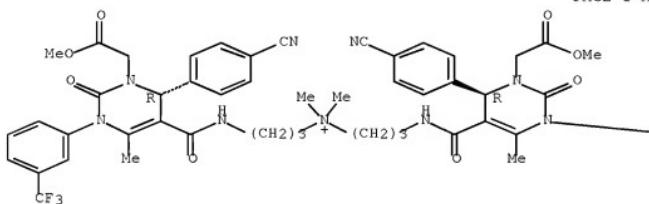


RN 917814-01-8 HCPLUS

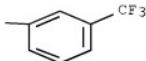
CN 1-Propanaminium, 3-[[[(4R)-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3-(2-methoxy-2-oxoethyl)-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]pyrimidinyl]carbonyl]amino]-N-[3-[[[(4R)-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3-(2-methoxy-2-oxoethyl)-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]pyrimidinyl]carbonyl]amino]propyl]-N,N-dimethyl-, iodide (1:1) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

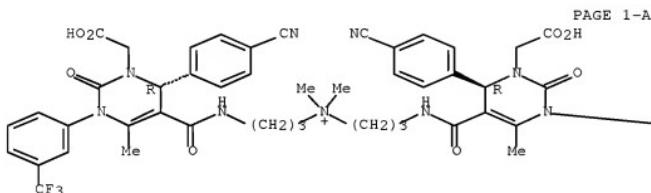


● I-

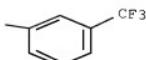


RN 917814-02-9 HCPLUS
 CN 1-Propanaminium, 3-[(4R)-3-(carboxymethyl)-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-5-pyrimidinyl]carbonyl]amino]-N-[3-[(4R)-3-(carboxymethyl)-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-5-pyrimidinyl]carbonyl]amino]propyl]-N,N-dimethyl-, chloride (1:1) (CA INDEX NAME)

Absolute stereochemistry.



● Cl⁻

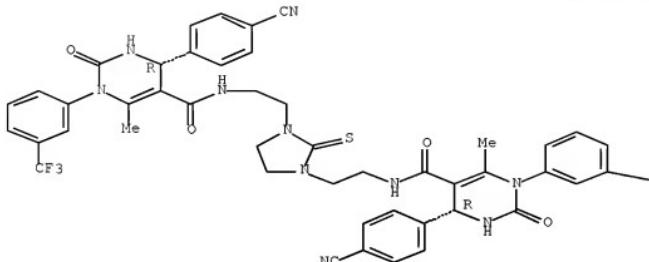


RN 917814-13-2 HCPLUS
 CN 5-Pyrimidinecarboxamide, N,N'-(2-thioxo-1,3-imidazolidinediyl)di-2,1-

ethanediyl]bis[4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, (4R,4'R)- (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

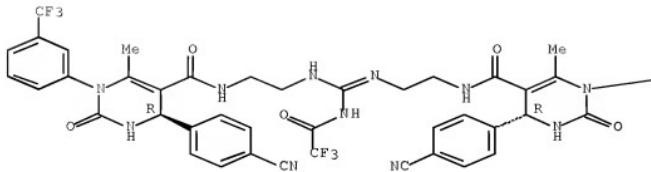
—CF₃

RN 917814-15-4 HCPLUS

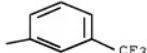
CN 5-Pyrimidinecarboxamide, N,N'-{[(2,2,2-trifluoroacetyl)carbonimidoyl]bis(imino-2,1-ethanediyl)]bis[4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, (4R,4'R)- (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

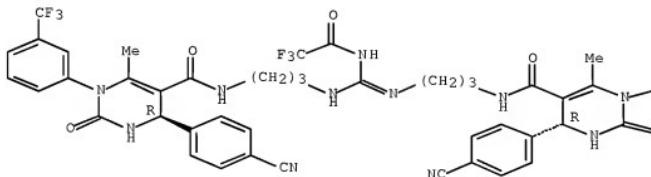


RN 917814-17-6 HCPLUS

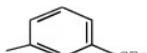
CN 5-Pyrimidinecarboxamide, N,N'-{[(2,2,2-trifluoroacetyl)carbonimidoyl]bis(i mino-3,1-propanediyl)]bis[4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, (4R,4'R)- (CA INDEX NAME)}

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

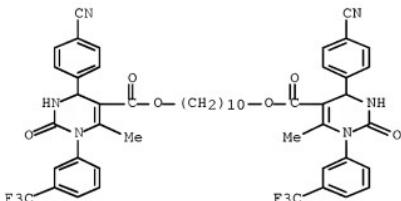
 \equiv

IT 917813-84-4P 917813-85-5P 917813-86-6P
 917813-97-7P 917813-98-9P 917813-91-3P
 917813-92-4P 917813-93-5P 917813-94-6P
 917813-95-7P 917813-96-8P 917814-00-7P
 917814-03-0P 917814-04-1P 917814-05-2P
 917814-06-3P 917814-07-4P 917814-08-5P
 917814-09-6P 917814-10-9P 917814-11-0P
 917814-12-1P 917814-14-3P 917814-16-5P
 917814-18-7P 917814-19-8P 917814-20-1P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of dihydropyrimidone multimers as human neutrophil elastase inhibitors)

RN 917813-84-4 HCPLUS

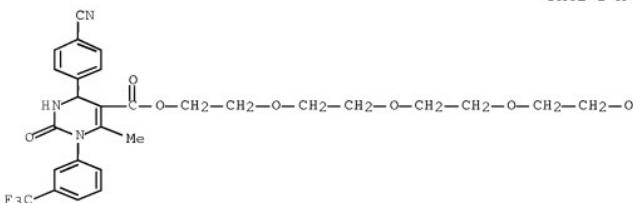
CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 5,5'-(1,10-decanediyl) ester (CA INDEX NAME)



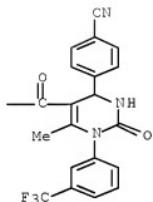
RN 917813-85-5 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 5,5'-[oxybis(2,1-ethanediyoxy-2,1-ethanediyl)] ester (CA INDEX NAME)

PAGE 1-A

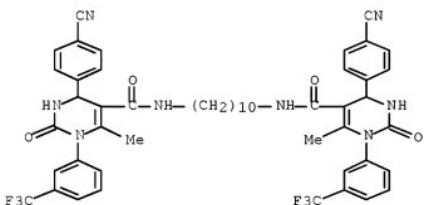


PAGE 1-B



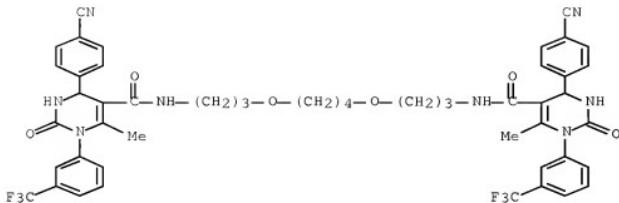
RN 917813-86-6 HCPLUS

CN 5-Pyrimidinecarboxamide, N,N'-1,10-decanediylbis[4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



RN 917813-87-7 HCPLUS

CN 5-Pyrimidinecarboxamide, N,N'-(1,4-butanediylbis(oxy-3,1-propanediyl)]bis[4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

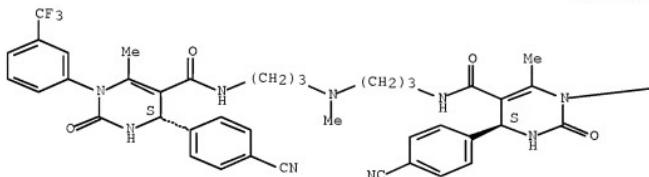


RN 917813-89-9 HCAPLUS

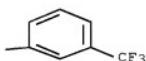
CN 5-Pyrimidinecarboxamide, N,N'-(methylimino)di-3,1-propanediyl bis[4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, (4S,4'S)- (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

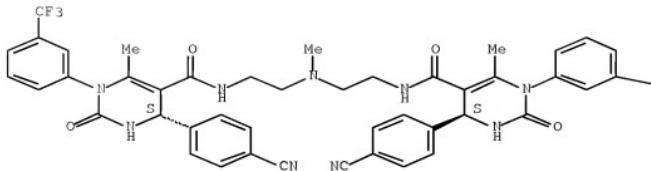


RN 917813-91-3 HCAPLUS

CN 5-Pyrimidinecarboxamide, N,N'-(methylimino)di-2,1-ethanediyl bis[4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, (4S,4'S)- (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

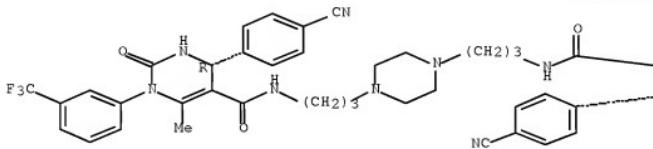
 ---CF_3

RN 917813-92-4 HCPLUS

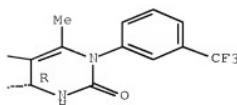
CN 5-Pyrimidinecarboxamide, N,N'-(1,4-piperazinediyl)bis[4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, (4R,4'R)- (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

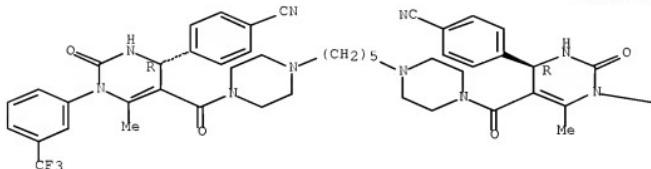


RN 917813-93-5 HCPLUS

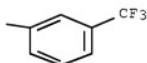
CN 5-Pyrimidinecarboxamide, N,N'-(1,5-pentanediyldi-4,1-piperazinediyl)bis[4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, (4R,4'R)- (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

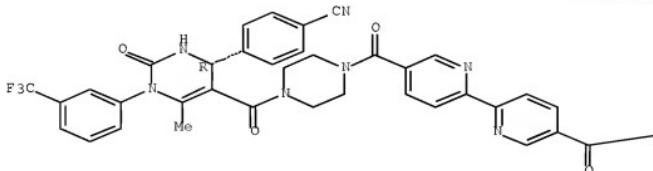


RN 917813-94-6 HCAPLUS

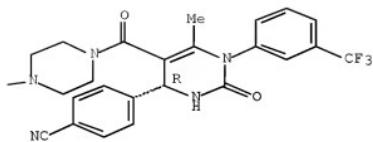
CN Benzonitrile, 4,4'-[{2,2'-bipyridine}-5,5'-diylbis[carbonyl-4,1-piperazinediylcarbonyl[(4R)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-(3-(trifluoromethyl)phenyl)-5,4-pyrimidinediyl]]]bis- (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

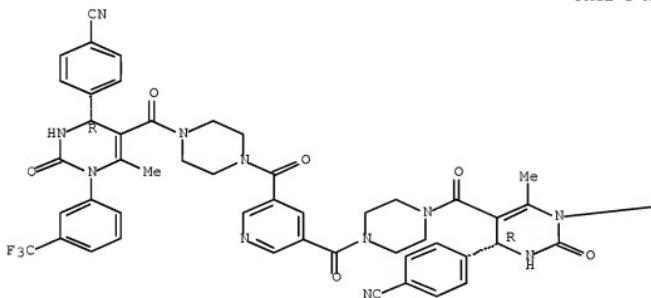


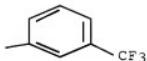
RN 917813-95-7 HCPLUS

CN Benzonitrile, 4,4'-[3,5-pyridinediylibis[carbonyl-4,1-piperazinediylibcarbonyl[(4R)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-(3-(trifluoromethyl)phenyl]-5,4-pyrimidinyl]]bis- (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

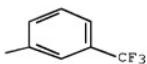
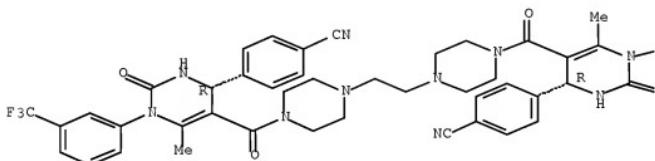




RN 917813-96-8 HCPLUS

CN Benzonitrile, 4,4'-[1,2-ethanediylbis[4,1-piperazinediylcarbonyl[(4R)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-5,4-pyrimidinediyl]]]bis- (CA INDEX NAME)

Absolute stereochemistry.

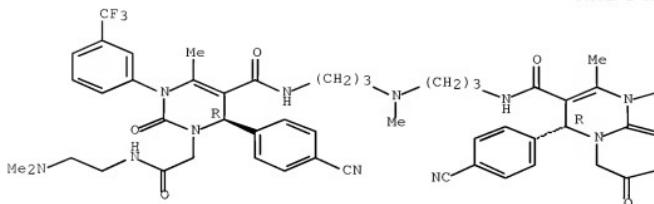


RN 917814-00-7 HCPLUS

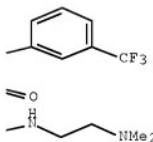
CN 1(2H)-Pyrimidineacetamide, 5,5'-[{(methylimino)bis(3,1-propanediyliminocarbonyl)]bis[6-(4-cyanophenyl)-N-[2-(dimethylamino)ethyl]-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, (6R,6'R)- (CA INDEX NAME)}

Absolute stereochemistry.

PAGE 1-A



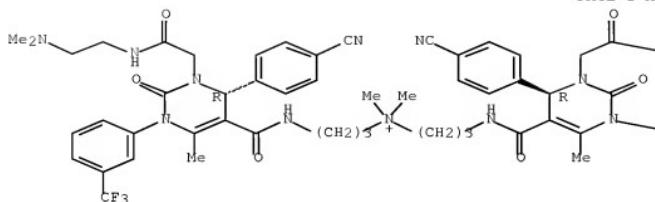
PAGE 1-B



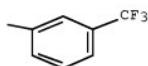
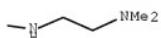
RN 917814-03-0 HCPLUS
 CN 1-Propanaminium, 3-[(4R)-4-(4-cyanophenyl)-3-[2-[(2-(dimethylamino)ethyl]amino]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-5-pyrimidinyl]carbonyl]amino]-N-[3-[(4R)-4-(4-cyanophenyl)-3-[2-[(2-(dimethylamino)ethyl]amino]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-5-pyrimidinyl]carbonyl]amino]propyl]-N,N-dimethyl-, chloride (1:1) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

● Cl⁻

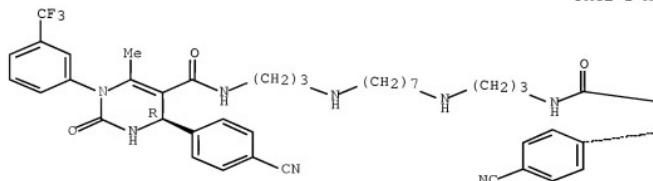
PAGE 1-B



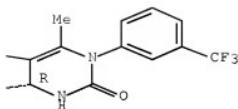
RN 917814-04-1 HCAPLUS
 CN 5-Pyrimidinecarboxamide, N,N'-[1,7-heptanediylbis(imino-3,1-propanediyl)]bis[4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, (4R,4'R)- (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

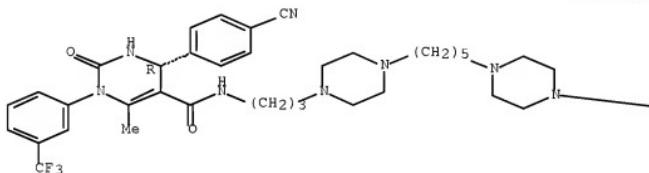


RN 917814-05-2 HCPLUS

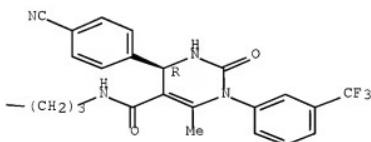
CN 5-Pyrimidinecarboxamide, N,N'-[1,5-pentanediyilbis(4,1-piperazinediyl-3,1-propanediyl)]bis[4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, (4R,4'R)- (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

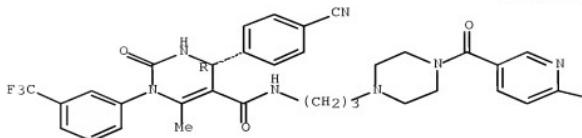


RN 917814-06-3 HCPLUS

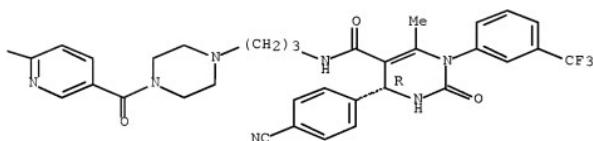
CN 5-Pyrimidinecarboxamide, N,N'-[{2,2'-bipyridine}-5,5'-diylbis(carbonyl-4,1-piperazinediyl-3,1-propanediyl)]bis[4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, (4R,4'R)- (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

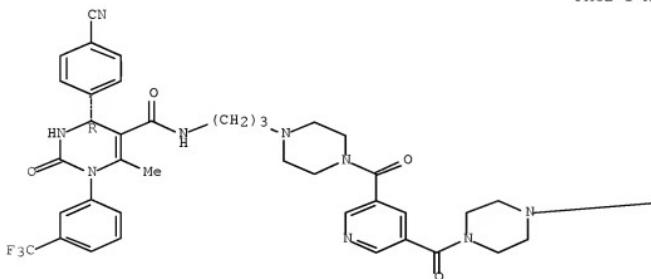


RN 917814-07-4 HCPLUS

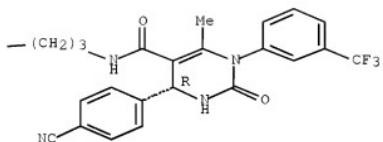
CN 5-Pyrimidinecarboxamide, N,N'-[3,5-pyridinediylbis(carbonyl-4,1-piperazinediyl-3,1-propanediyl)]bis[4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, (4R,4'R)- (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

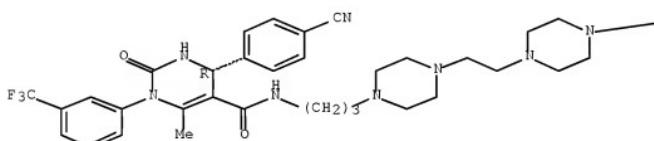


RN 917814-08-5 HCPLUS

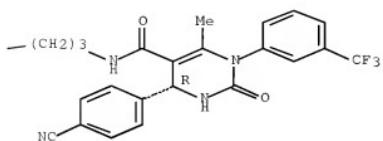
CN 5-Pyrimidinecarboxamide, N,N'-(1,2-ethanediylbis(4,1-piperazinediyl-3,1-propanediyl))bis[4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, (4R,4'R)- (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

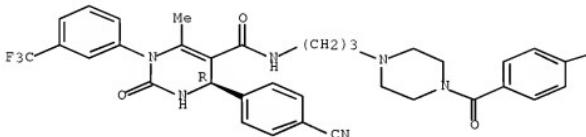


RN 917814-09-6 HCAPLUS

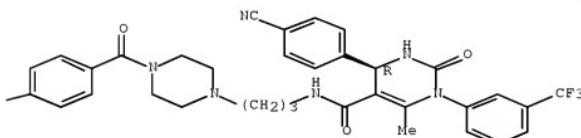
CN 5-Pyrimidinecarboxamide, N,N'-[{1,1'-biphenyl}-4,4'-diyl]bis(carbonyl-4,1-piperazinediyl-3,1-propanediyl)]bis[4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, (4R,4'R)- (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

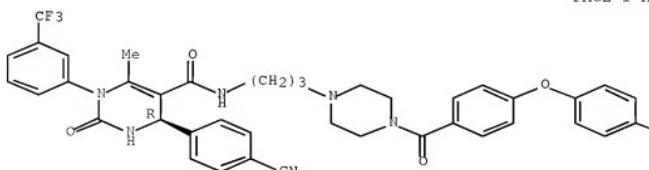


RN 917814-10-9 HCAPLUS

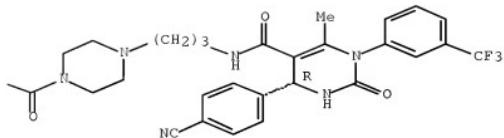
CN 5-Pyrimidinecarboxamide, N,N'-[oxybis(4,1-phenylene)carbonyl-4,1-piperazinediyl-3,1-propanediyl)]bis[4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, (4R,4'R)- (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

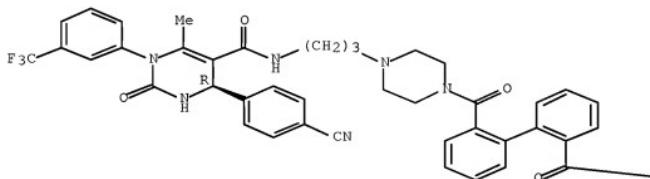


RN 917814-11-0 HCPLUS

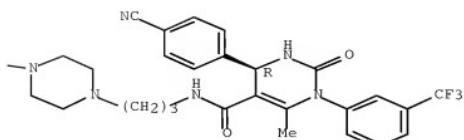
CN 5-Pyrimidinecarboxamide, N,N'-[{[1,1'-biphenyl]-2,2'-diyl}bis(carbonyl-4,1-piperazinediyl-3,1-propanediyl)]bis[4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, (4R,4'R)- (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

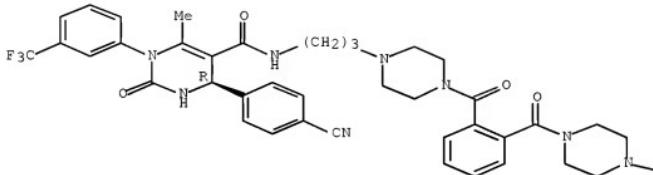


RN 917814-12-1 HCPLUS

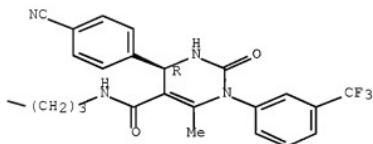
CN 5-Pyrimidinecarboxamide, N,N'-[1,4-phenylenebis(carbonyl-4,1-piperazinediyl-3,1-propanediyl)]bis[4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, (4R,4'R)- (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

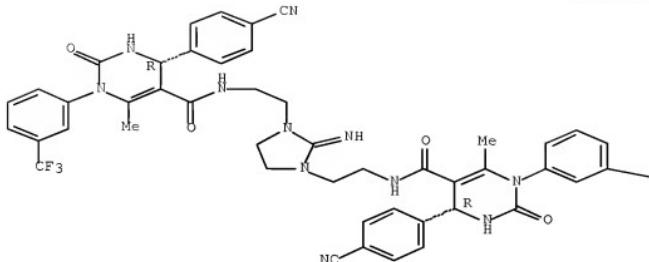


RN 917814-14-3 HCPLUS

CN 5-Pyrimidinecarboxamide, N,N'-[{(2-imino-1,3-imidazolidinediyl)di-2,1-ethanediyil]bis[4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, (4R,4'R)- (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



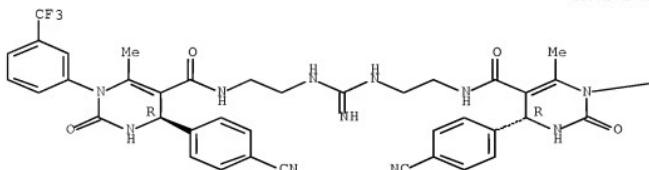
PAGE 1-B

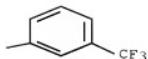
—CF₃

RN 917814-16-5 HCPLUS
 CN 5-Pyrimidinecarboxamide, N,N'-[carbonimidoylbis(imino-2,1-ethanediyl)]bis[4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, (4R,4'R)- (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

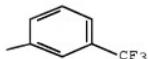
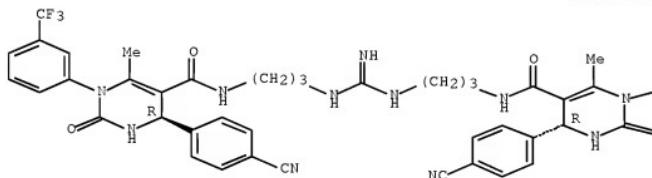




RN 917814-18-7 HCAPLUS

CN 5-Pyrimidinecarboxamide, N,N'-(carbonimidoylbis(imino-3,1-propanediyl))bis(4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, (4R,4'R)- (CA INDEX NAME)

Absolute stereochemistry.

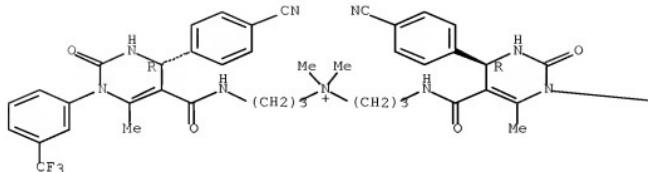
 $\equiv \text{O}$

RN 917814-19-8 HCAPLUS

CN 1-Propanaminium, 3-[[[(4R)-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-5-pyrimidinyl]carbonyl]amino]-N-[3-[[[(4R)-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-5-pyrimidinyl]carbonyl]amino]propyl]-N,N-dimethyl-, iodide (1:1) (CA INDEX NAME)

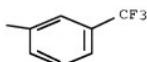
Absolute stereochemistry.

PAGE 1-A



● I-

PAGE 1-B

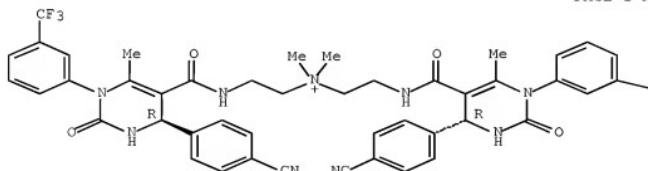


RN 917814-20-1 HCPLUS

CN Ethanaminium, 2-[[[(4R)-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]5-pyrimidinyl]carbonyl]amino]-N-[2-[[[(4R)-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]5-pyrimidinyl]carbonyl]amino]ethyl]-N,N-dimethyl-, iodide (1:1) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



● I-

~~—CF₃~~

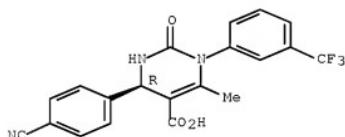
IT 864228-16-0P

RL: PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of dihydropyrimidone multimers as human neutrophil elastase inhibitors)

RN 864228-16-0 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, (4R)- (CA INDEX NAME)

Absolute stereochemistry.

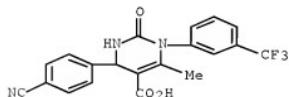


IT 671775-95-4

RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of dihydropyrimidone multimers as human neutrophil elastase inhibitors)

RN 671775-95-4 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



IT 864151-33-7P 904958-42-5P 917814-21-2P

917814-21-3P 917814-23-4P 917814-24-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

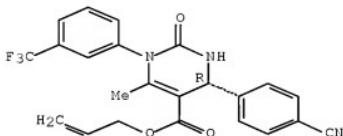
(preparation of dihydropyrimidone multimers as human neutrophil elastase

(inhibitors)

RN 864151-33-7 HCPLUS

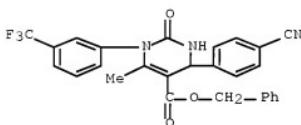
CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-propen-1-yl ester, (4R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 904958-42-5 HCPLUS

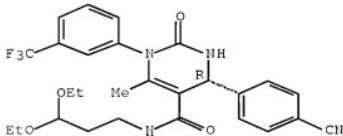
CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, phenylmethyl ester (CA INDEX NAME)



RN 917814-21-2 HCPLUS

CN 5-Pyrimidinecarboxamide, 4-(4-cyanophenyl)-N-(3,3-diethoxypropyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, (4R)- (CA INDEX NAME)

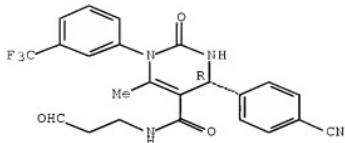
Absolute stereochemistry.



RN 917814-22-3 HCPLUS

CN 5-Pyrimidinecarboxamide, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-N-(3-oxopropyl)-1-[3-(trifluoromethyl)phenyl]-, (4R)- (CA INDEX NAME)

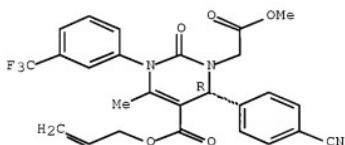
Absolute stereochemistry.



RN 917814-23-4 HCPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-[(2-propanoyloxy)carbonyl]-3-[3-(trifluoromethyl)phenyl]-, methyl ester, (6R)- (CA INDEX NAME)

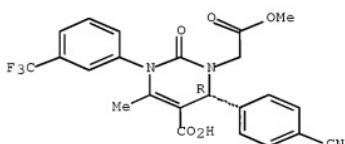
Absolute stereochemistry.



RN 917814-24-5 HCPLUS

CN 1(2H)-Pyrimidineacetic acid, 5-carboxy-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1-methyl ester, (6R)- (CA INDEX NAME)

Absolute stereochemistry.



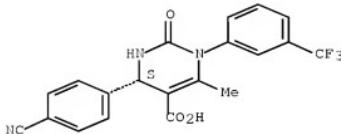
IT 917814-25-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of dihydropyrimidone multimers as human neutrophil elastase inhibitors)

RN 917814-25-6 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, (4S)- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L57 ANSWER 2 OF 15 HCPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 2
 ACCESSION NUMBER: 2006:796025 HCPLUS Full-text
 DOCUMENT NUMBER: 145:211067
 TITLE: Multimers of tetrahydropyrimidinone compounds as elastase inhibitors and their preparation, pharmaceutical compositions, and use for treatment of respiratory diseases
 INVENTOR(S): Finch, Harry; Edwards, Christine; Ray, Nicholas Charles; O'Connor, Elizabeth Anne; Fitzgerald, Mary F.
 PATENT ASSIGNEE(S): Argenta Discovery Ltd, UK
 SOURCE: PCT Int. Appl., 132 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|--------------|
| WO 2006082412 | A2 | 20060810 | WO 2006-GB361 | 20060203 <-- |
| WO 2006082412 | A3 | 20061012 | | |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| AU 2006210730 | A1 | 20060810 | AU 2006-210730 | 20060203 <-- |
| CA 2595801 | A1 | 20060810 | CA 2006-2595801 | 20060203 <-- |
| EP 1856059 | A2 | 20071121 | EP 2006-709612 | 20060203 <-- |
| R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR | | | | |
| IN 2007DN05905 | A | 20070817 | IN 2007-DN5905 | 20070727 <-- |

CN 101151252 A 20080326 CN 2006-80009856 20070926 <--
 PRIORITY APPLN. INFO.: GB 2005-2258 A 20050203 <--
 OTHER SOURCE(S): MARPAT 145:211067 WO 2006-GB361 W 20060203
 ED Entered STN: 11 Aug 2006
 GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB A compound of formula I is useful in therapy, e.g. of respiratory diseases. Compds. of formula I wherein L is a linker; each A are independently (un)substituted (hetero)aryl; D is O or S; each Y1 - Y5 are independently CH, CR3, CR6 or N, with the proviso that one of them is CR3, one CR6 and not more than two N per ring; each R3 are independently H, halo, NO2, CN, (un)substituted C1-6 alkyl, OH, or (un)substituted C1-6 alkoxy; each R4 are independently COCF3, (un)substituted C1-6 alkylcarbonyl, (un)substituted C1-6 alkoxycarbonyl, (un)substituted C1-6 alkenyloxycarbonyl, hydroxycarbonyl, CONH2 and derivs., (un)substituted (hetero)acyl, etc.; each R5 are independently (un)substituted C1-4 alkyl or amino; each R6 are independently halo, NO2, CN, (un)substituted C1-6 alkyl, OH, or (un)substituted C1-6 alkoxy; and their pharmaceutically acceptable salts, solvates or N-oxides thereof are claimed. Example compound II was prepared by N-alkylation of compound III with 1,12-dibromododecane. The invention compds. were evaluated for their elastase inhibitory activity. The tested compds. were shown to have desirable HNE inhibitory activity (no data).

IT 904957-71-7P 904957-72-6P 904957-86-4P
 904958-07-2P

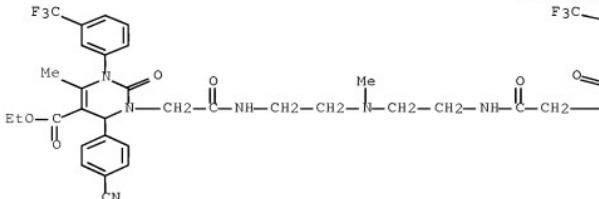
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
 (drug candidate and intermediate; preparation of multimers of tetrahydropyrimidinone compds. as elastase inhibitors useful in the treatment of respiratory diseases)

RN 904957-71-7 HCPLUS

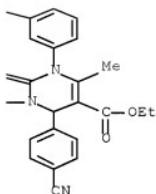
CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[[2-[[2-[(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl)methylamino]ethyl]amino]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)

PAGE 1-A

F3C—



PAGE 1-B

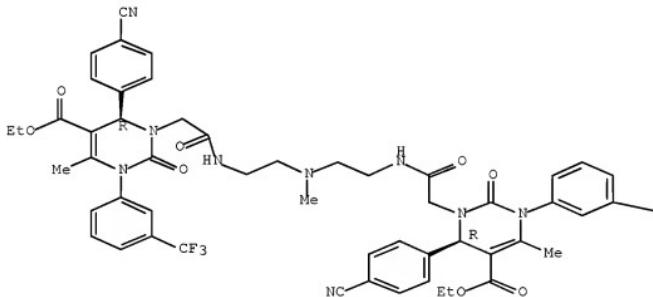


BN 904957-72-8 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[2-[2-[2-[2-[(6R)-6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl]methylamino]ethyl]amino]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester, (4R)- (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

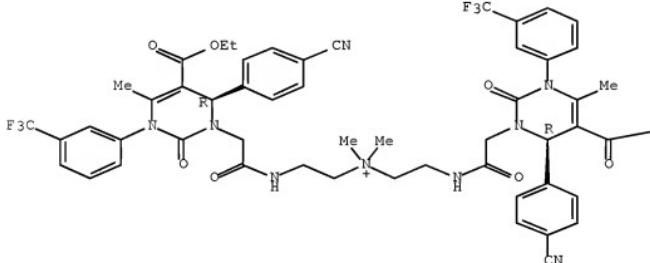


---CF_3

RN 904957-86-4 HCPLUS

CN Ethanaminium, 2-[(2-[(6R)-6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]-N-[2-[(2-[(6R)-6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl]-N,N-dimethyl-, iodide (1:1) (CA INDEX NAME)

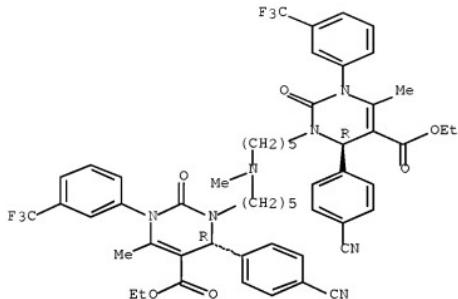
Absolute stereochemistry.

 ---OEt $\bullet \text{I}^-$

RN 904958-07-2 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-(methylimino)di-5,1-pentanediyil]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester, (6R,6'R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



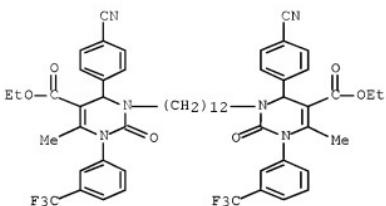
IT 904957-62-6P 904957-63-7P 904957-64-8P
 904957-65-9P 904957-66-0P 904957-67-1P
 904957-68-2P 904957-69-3P 904957-70-6P
 904957-73-5P 904957-74-0P 904957-75-1P
 904957-76-2P 904957-77-3P 904957-78-4P
 904957-79-5P 904957-80-6P 904957-81-9P
 904957-83-1P 904957-84-2P 904957-85-3P
 904957-87-5P 904957-88-6P 904957-89-7P
 904957-90-0P 904957-91-1P 904957-92-2P
 904957-93-3P 904957-94-4P 904957-95-5P
 904957-96-6P 904957-97-7P 904957-98-8P
 904957-99-9P 904958-00-5P 904958-01-6P
 904958-02-7P 904958-03-8P 904958-04-9P
 904958-05-0P 904958-06-1P 904958-08-3P
 904958-09-4P 904958-10-7P 904958-11-8P
 904958-12-9P 904958-13-0P 904958-14-1P
 904958-15-2P 904958-16-3P 904958-17-4P
 904958-18-5P 904958-19-6P 904958-20-9P
 904958-21-0P 904958-22-1P 904958-23-2P
 904958-24-3P 904958-25-4P 904958-26-5P
 904958-27-6P 904958-28-7P 904958-30-1P
 904958-31-2P 904958-32-3P 904958-33-4P
 904958-34-5P 904958-37-8P 904958-39-0P
 904958-41-4P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of multimers of tetrahydropyrimidinone compds.
as elastase inhibitors useful in the treatment of respiratory diseases)

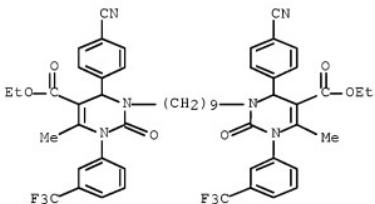
RN 904957-62-6 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-(1,12-dodecanediyl)bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)



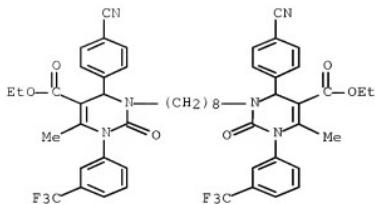
RN 904957-63-7 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-(1,9-nonanediyl)bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)



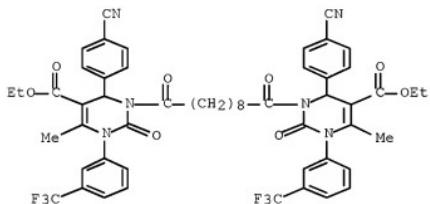
RN 904957-64-8 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-(1,8-octanediyl)bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)



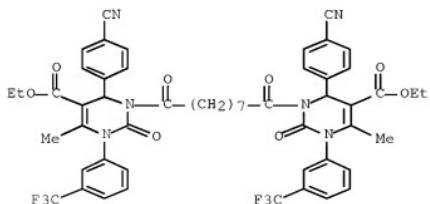
RN 904957-65-9 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-(1,10-dioxo-1,10-decanediyl)bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)



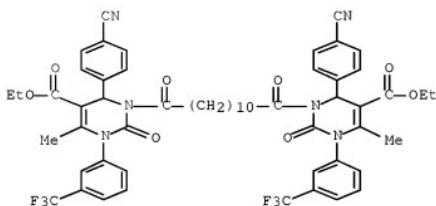
RN 904957-66-0 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-(1,9-dioxo-1,9-nonanediyyl)bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)



RN 904957-67-1 HCPLUS

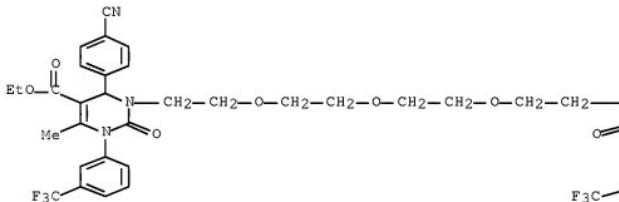
CN 5-Pyrimidinecarboxylic acid, 1,1'-(1,12-dioxo-1,12-dodecanediyl)bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)



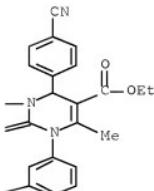
RN 904957-68-2 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-[oxybis(2,1-ethanediyoxy-2,1-ethanediyl)]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

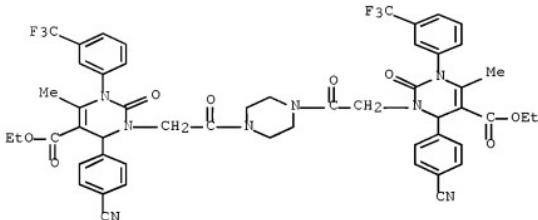


PAGE 1-B



RN 904957-69-3 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[4-[2-[6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]-1-piperazinyl]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)

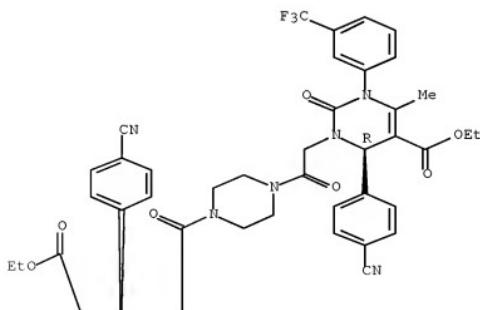


RN 904957-70-6 HCPLUS

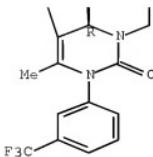
CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[4-[2-[(6R)-6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]-1-piperazinyl]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester, (4R)- (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



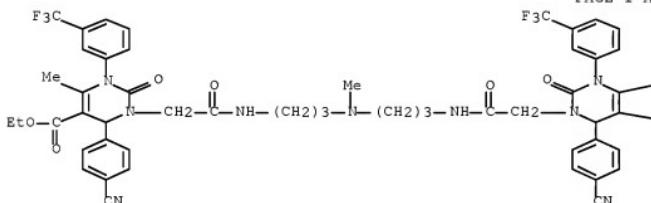
PAGE 2-A



RN 904957-73-9 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[3-[2-[6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]phenyl]-1(2H)-pyrimidinyl]acetyl]aminolpropyl]methylamino]propyl]amino]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)

PAGE 1-A



PAGE 1-B

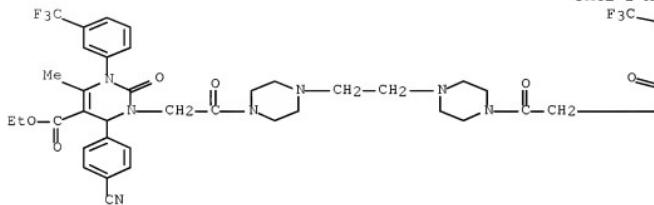


RN 904957-74-0 HCAPLUS

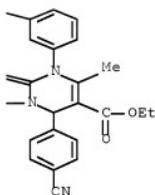
CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[4-[2-[4-[2-[6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]phenyl]-1(2H)-pyrimidinyl]acetyl]-1-piperazinyl]ethyl]-1-

piperazinyl]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)

PAGE 1-A
F₃C—



PAGE 1-B

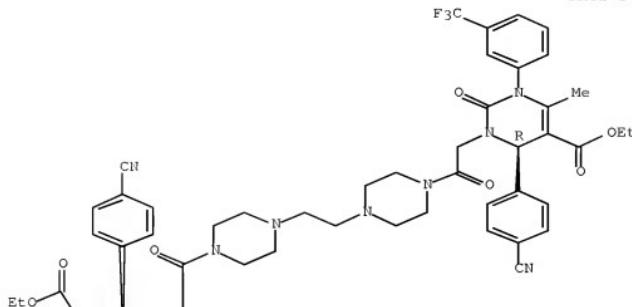


RN 904957-75-1 HCPLUS

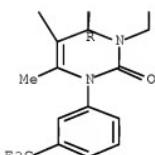
CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[4-[2-[4-[(6R)-6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]phenyl]-1(2H)-pyrimidinyl]acetyl]-1-piperazinyl]ethyl]-1-piperazinyl]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester, (4R)- (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A

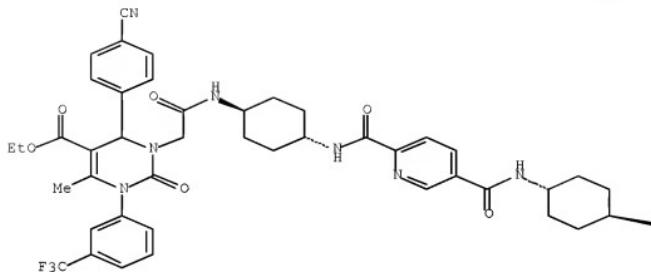


RN 904957-76-2 HCPLUS

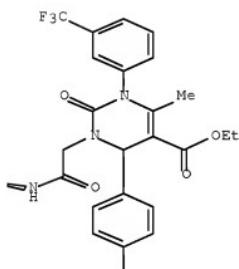
CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[[trans-4-[[[5-
[[trans-4-[[2-[6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-
2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]cyclohe-
xyl]amino]carbonyl]-2-pyridinyl]carbonyl]amino]cyclohexyl]amino]-2-
oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-
, ethyl ester (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



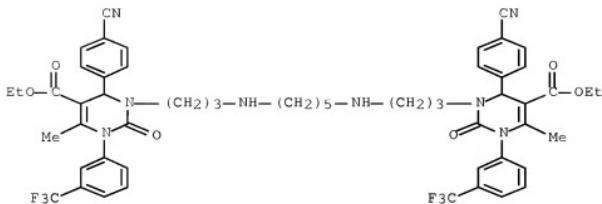
PAGE 1-B



PAGE 2-B

CN

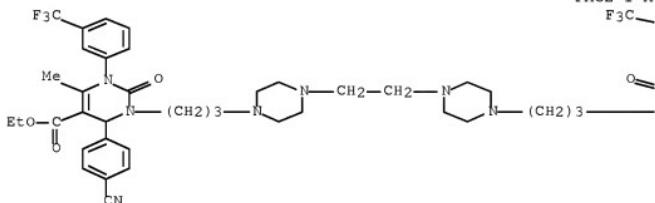
RN 904957-77-3 HCPLUS
 CN 5-Pyrimidinecarboxylic acid, 1,1'-[1,5-pentanediylibis(imino-3,1-propanediyl)]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-(3-(trifluoromethyl)phenyl)-, diethyl ester, (6R,6'R)-(9CI) (CA INDEX NAME)



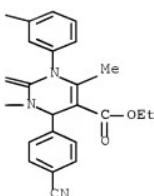
RN 904957-78-4 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-[1,2-ethanediyliobis(4,1-piperazinediyl)-3,1-propanediyl]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

F3C

PAGE 1-B



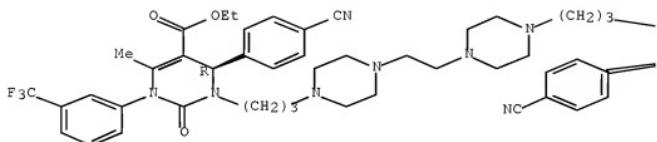
RN 904957-79-5 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-[1,2-ethanediyliobis(4,1-piperazinediyl)-

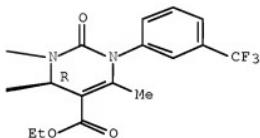
3,1-propanediyl)]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]phenyl]-, diethyl ester, (6R,6'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

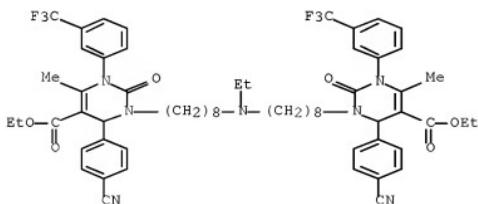


PAGE 1-B



RN 904957-80-8 HCPLUS

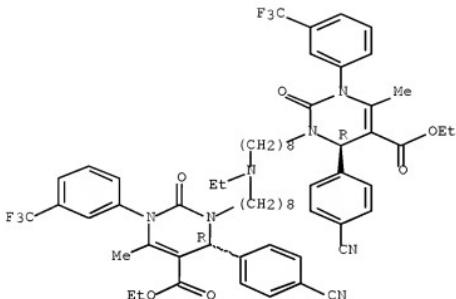
CN 5-Pyrimidinecarboxylic acid, 1,1'-(ethylimino)di-8,1-octanediyil]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)



RN 904957-81-9 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-(ethylimino)di-8,1-octanediyil]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester, (6R,6'R)- (CA INDEX NAME)

Absolute stereochemistry.



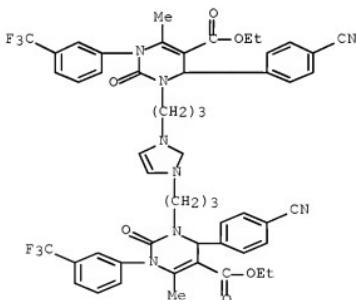
RN 904957-83-1 HCPLUS

CN 1H-Imidazolium, 1,3-bis[3-[6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]propyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 904957-82-0

CMF C53 H49 F6 N8 O6

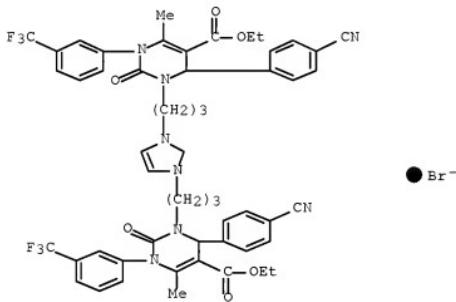


ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

CM 2

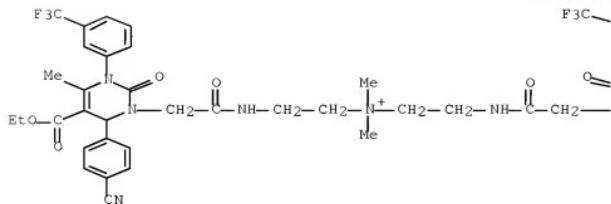
CRN 14477-72-6
CMF C2 F3 O2

RN 904957-84-2 HCPLUS
 CN 1H-Imidazolium, 1,3-bis[3-[6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]propyl]-, bromide (1:1) (CA INDEX NAME)



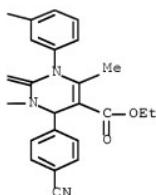
ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 904957-85-3 HCPLUS
 CN Ethanaminium, 2-[[2-[6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]-N-[2-[[2-[6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]ethyl]-N,N-dimethyl-, iodide (1:1) (CA INDEX NAME)

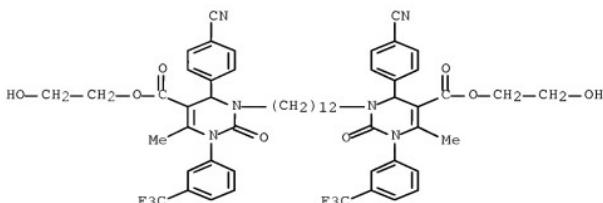
PAGE 1-A
F3C-

● I-

PAGE 1-B



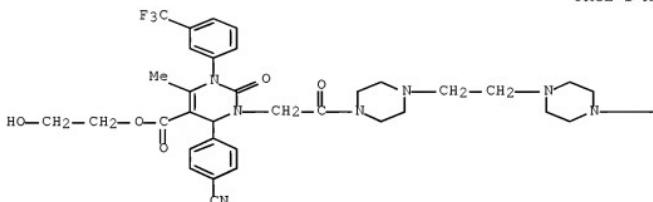
RN 904957-87-5 HCAPLUS
 CN 5-Pyrimidinecarboxylic acid, 1,1'-(1,12-dodecanediyl)bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, bis(2-hydroxyethyl) ester (9CI) (CA INDEX NAME)



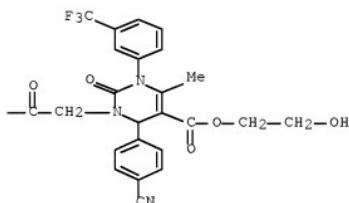
RN 904957-88-6 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[4-[2-[4-[2-[6-(4-cyanophenyl)-3,6-dihydro-5-[(2-hydroxyethoxy)carbonyl]-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]-1-piperazinyl]ethyl]-1-piperazinyl]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-hydroxyethyl ester (CA INDEX NAME)

PAGE 1-A



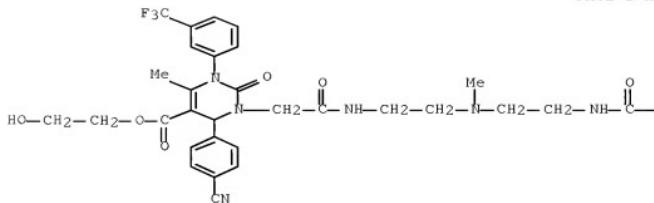
PAGE 1-B



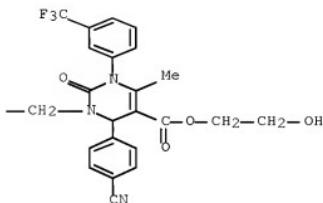
RN 904957-89-7 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[4-[2-[4-[2-[6-(4-cyanophenyl)-3,6-dihydro-5-[(2-hydroxyethoxy)carbonyl]-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-hydroxyethyl ester (CA INDEX NAME)

PAGE 1-A



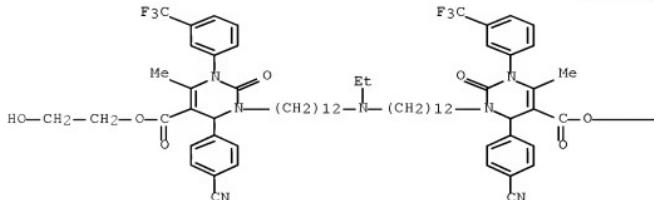
PAGE 1-B



RN 904957-90-0 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-[{ethylimino}di-12,1-dodecanediyl]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, bis(2-hydroxyethyl) ester (9CI) (CA INDEX NAME)

PAGE 1-A

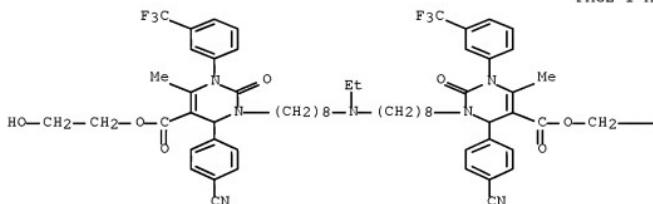


PAGE 1-B

 $\text{---CH}_2\text{---CH}_2\text{---OH}$

RN 904957-91-1 HCAPLUS
 CN 5-Pyrimidinecarboxylic acid, 1,1'-(ethylimino)di-8,1-octanediyil]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, bis(2-hydroxyethyl) ester (9CI) (CA INDEX NAME)

PAGE 1-A

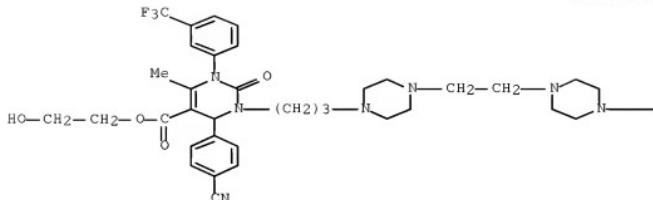


PAGE 1-B

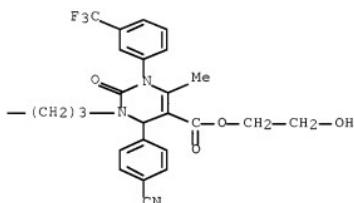
 $\text{---CH}_2\text{---OH}$

RN 904957-92-2 HCAPLUS
 CN 5-Pyrimidinecarboxylic acid, 1,1'-(1,2-ethanediyl)bis(4,1-piperazinediyil-3,1-propanediyl)bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, bis(2-hydroxyethyl) ester (9CI) (CA INDEX NAME)

PAGE 1-A



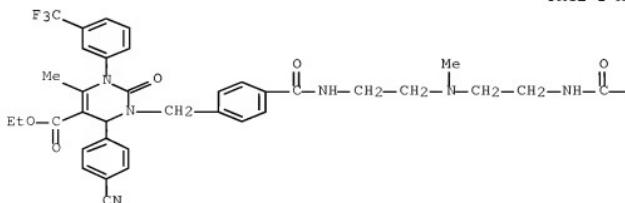
PAGE 1-B



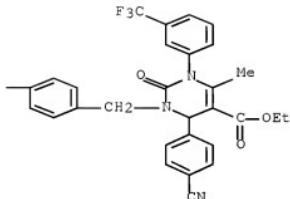
RN 904957-93-3 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[(4-((2-methyl-3-(trifluoromethyl)phenyl)amino)carbonyl)phenyl]methyl]-1(2H)-pyrimidinyl)methyl]benzoyl]amino]ethyl]methylenamino]ethyl]amino]carbonyl]phenyl]methyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-(3-(trifluoromethyl)phenyl)-, ethyl ester (CA INDEX NAME)

PAGE 1-A



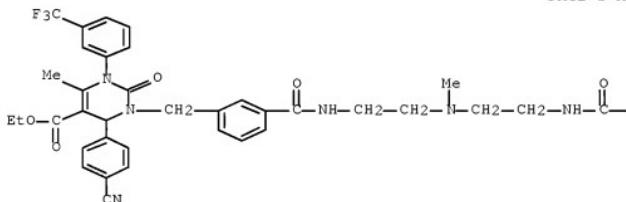
PAGE 1-B

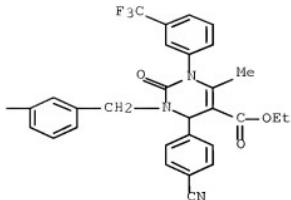


RN 904957-94-4 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[[3-[[2-[[2-[[3-[[6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]benzoyl]amino]ethyl]methylamino]ethyl]amino]carbonyl]phenyl)methyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)

PAGE 1-A

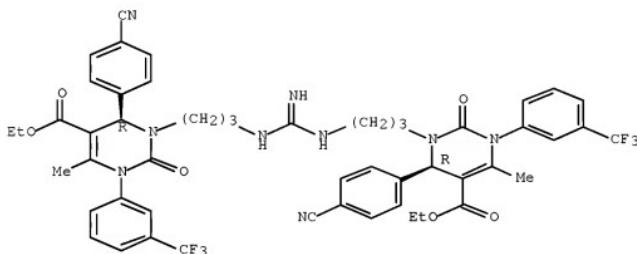




RN 904957-95-5 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-(carbonimidoylbis(imino-3,1-propanediyl))bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester, (6R,6'R)- (9CI) (CA INDEX NAME)

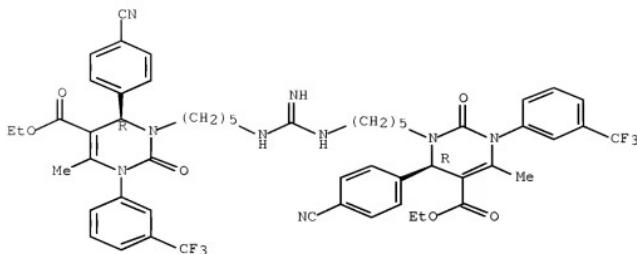
Absolute stereochemistry.



RN 904957-96-6 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-(carbonimidoylbis(imino-5,1-pentanediy))bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester, (6R,6'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

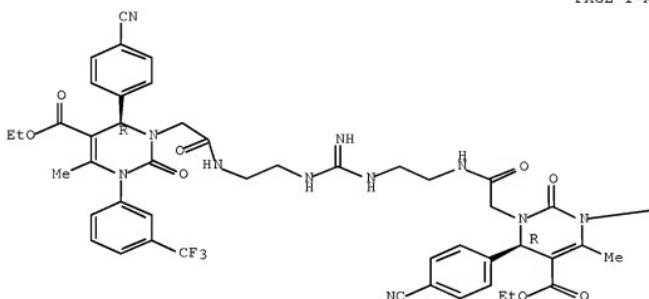


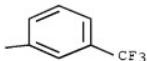
RN 904957-97-7 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-(7-imino-2,12-dioxo-3,6,8,11-tetraaza-1,13-tridecanediyl)bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester, (6R,6'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

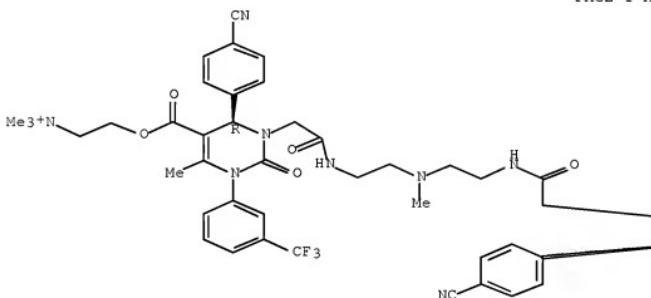


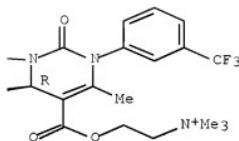


RN 904957-98-8 HCPLUS

CN Ethanaminium, 2,2'-[{(methylimino)bis[2,1-ethanediyl]imino(2-oxo-2,1-ethanediyl)][(6R)-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1,5(2H)-pyrimidinediyl]carbonyloxy]]bis[N,N,N-trimethyl-, diiodide (9CI) (CA INDEX NAME)

Absolute stereochemistry.

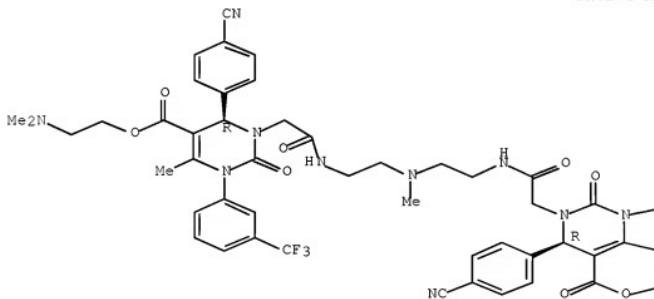


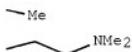
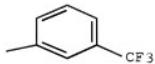


RN 904957-99-9 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[(2-[(2-[(6R)-6-(4-cyanophenyl)-5-[(2-(dimethylamino)ethoxy]carbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl]methylaminol]ethyl]amino]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-(dimethylamino)ethyl ester, (4R)- (CA INDEX NAME)

Absolute stereochemistry.

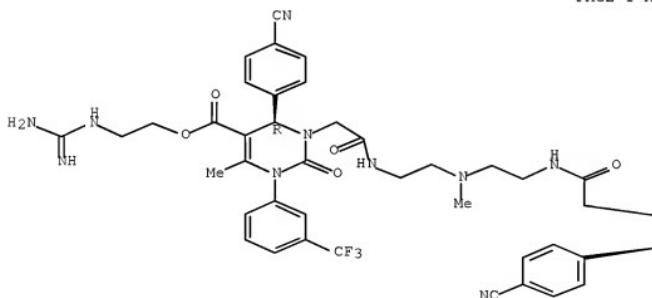


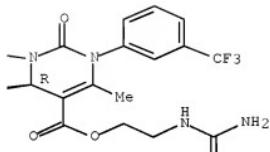


RN 904958-00-5 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 3-[2-[(2-[(2-[(6R)-5-[(2-[(aminoiminomethyl)amino]ethoxy)carbonyl]-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl]methylamino]ethyl]amino]-2-oxoethyl]-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-[(aminoiminomethyl)amino]ethyl ester, (4R)-(CA INDEX NAME)

Absolute stereochemistry.

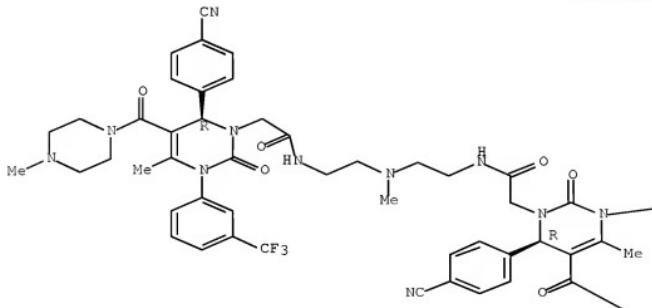


 H_{NH}

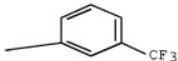
RN 904958-01-6 HCPLUS

CN 1(2H)-Pyrimidineacetamide, N,N'-(methylimino)di-2,1-ethanediyl]bis[6-(4-cyanophenyl)-3,6-dihydro-4-methyl-5-[(4-methyl-1-piperazinyl)carbonyl]-2-oxo-3-[3-(trifluoromethyl)phenyl]-, (6R,6'R)-(9CI) (CA INDEX NAME)

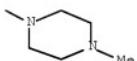
Absolute stereochemistry.



PAGE 1-B



PAGE 2-A

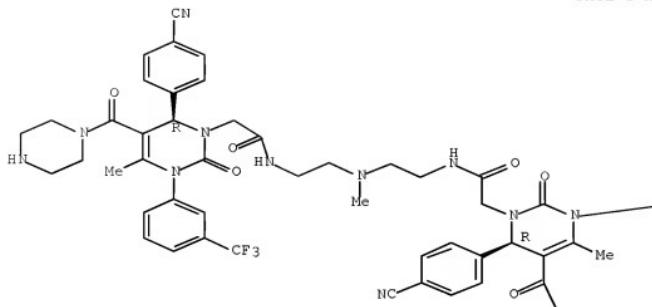


PAGE 2-B

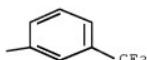
RN 904958-02-7 HCPLUS
CN 1(2H)-Pyrimidineacetamide, N,N'-(methylimino)di-2,1-ethanediyl]bis[6-(4-cyanophenyl)-3,6-dihydro-4-methyl-5-(1-piperazinylcarbonyl)-2-oxo-3-(3-(trifluoromethyl)phenyl]-, (6R,6'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

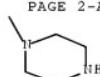
PAGE 1-A



PAGE 1-B

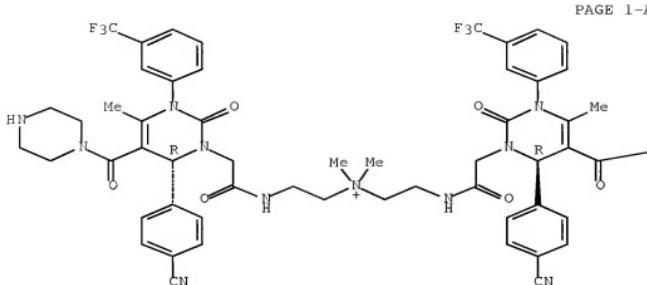


PAGE 2-A

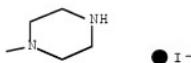


RN 904958-03-8 HCAPLUS
 CN Ethanaminium, 2-[(2-[(6R)-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-(1-piperazinylcarbonyl)-3-(3-(trifluoromethyl)phenyl)-1(2H)-pyrimidinyl]acetyl)amino]-N-[2-[(2-[(6R)-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-(1-piperazinylcarbonyl)-3-(3-(trifluoromethyl)phenyl)-1(2H)-pyrimidinyl]acetyl)amino]ethyl]-N,N-dimethyl-, iodide (1:1) (CA INDEX NAME)

Absolute stereochemistry.

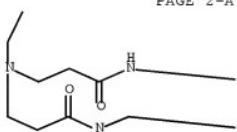
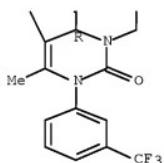
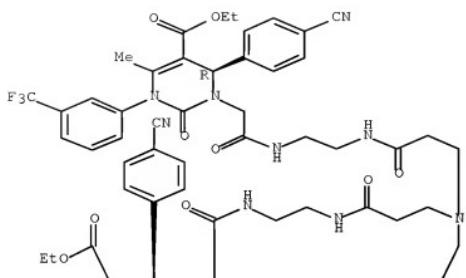


PAGE 1-B

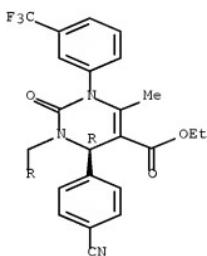
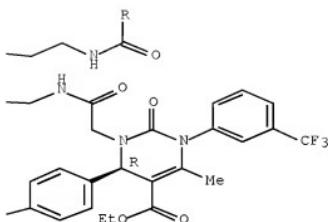


RN 904958-04-9 HCAPLUS
 CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[22-[(6R)-6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]-10,13-bis[3-[(2-[(2-[(6R)-6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl]amino]-3-oxopropyl]-2,7,16,21-tetraoxo-3,6,10,13,17,20-hexaazadocos-1-yl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester, (4R)- (CA INDEX NAME)

Absolute stereochemistry.



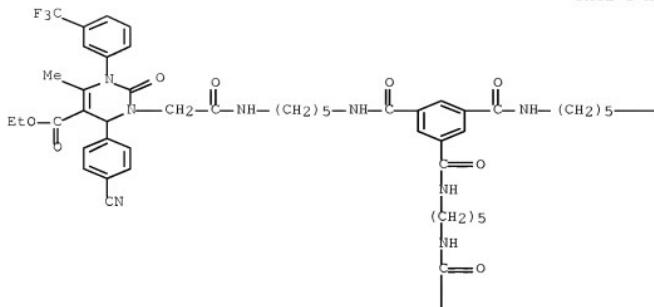
NC-



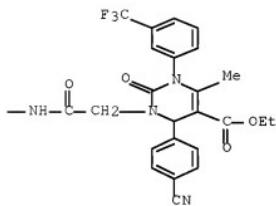
RN 904958-05-0 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 3-[2-[[5-[[3,5-bis[[[5-[[2-[6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]aminopentyl]amino]carbonyl]benzoyl]amino]pentyl]amino]-2-oxoethyl]-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)

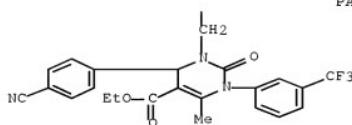
PAGE 1-A



PAGE 1-B



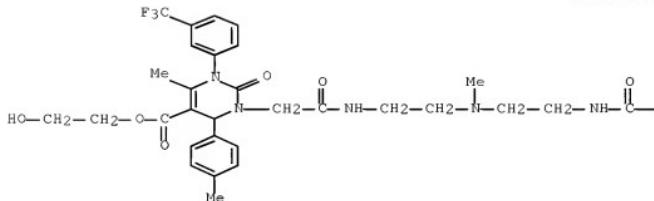
PAGE 2-A



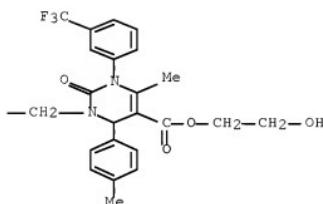
RN 904958-06-1 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 3-[2-[[2-[[2-[(2-[3,6-dihydro-5-[(2-hydroxyethoxy)carbonyl]-4-methyl-6-(4-methylphenyl)-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl]methylamino]ethyl]amino]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-4-(4-methylphenyl)-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-hydroxyethyl ester (CA INDEX NAME)

PAGE 1-A



PAGE 1-B

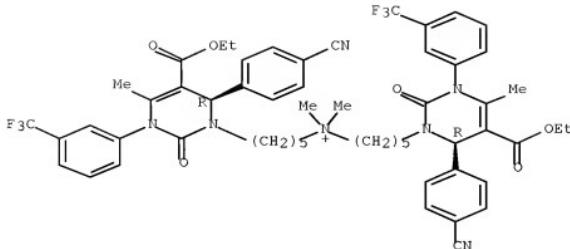


RN 904958-08-3 HCAPLUS

CN 1(2H)-Pyrimidinepentanaminium, 6-(4-cyanophenyl)-N-[5-[(6R)-6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]pentyl]-5-(ethoxycarbonyl)-3,6-dihydro-N,N,4-trimethyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, iodide (1:1), (6R)- (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

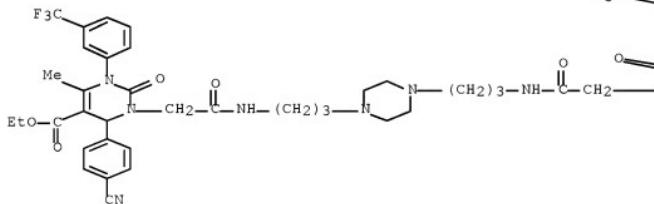


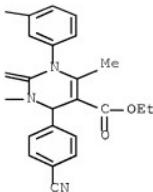
PAGE 2-A

● I -

RN 904958-09-4 HCAPLUS
 CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[3-[4-[3-[2-[6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]propyl]-1-piperazinylpropylamino]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)

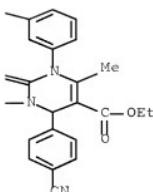
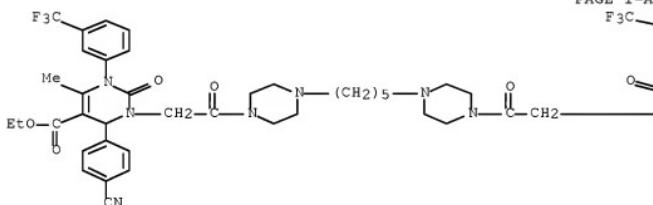
PAGE 1-A

F₃C—



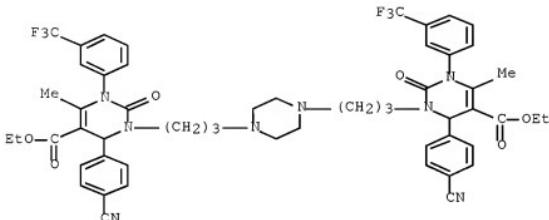
RN 904958-10-7 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[4-[5-[4-[2-[6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]-1-piperazinyl]pentyl]-1-piperazinyl]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



RN 904958-11-8 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-(1,4-piperazinediyldi-3,1-propanediyl)bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)

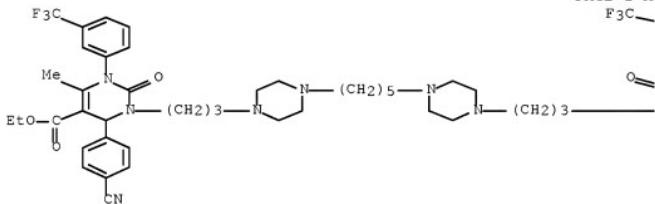


RN 904958-12-9 HCAPLUS

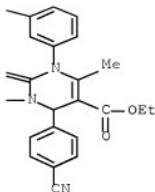
CN 5-Pyrimidinecarboxylic acid, 1,1'-(1,5-pentanediylbis(4,1-piperazinediyil-3,1-propanediyl))bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

F3C—



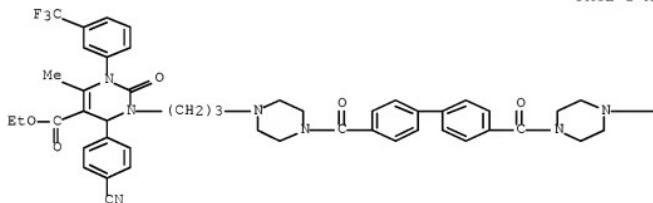
PAGE 1-B



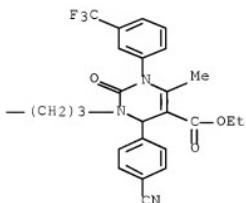
RN 904958-13-0 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-(1,1'-biphenyl)-4,4'-diylbis(carbonyl-4,1-piperazinediyl-3,1-propanediyl)bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



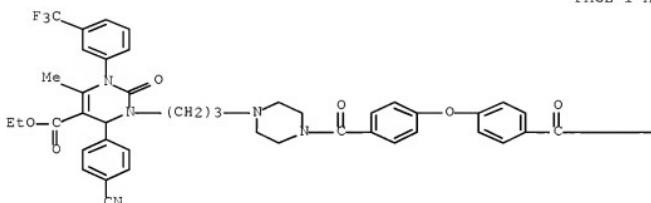
PAGE 1-B



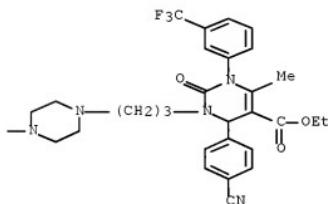
RN 904958-14-1 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-(oxybis(4,1-phenylene carbonyl-4,1-piperazinediyl-3,1-propanediyl))bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



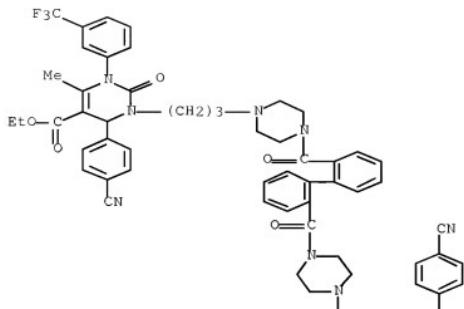
PAGE 1-B



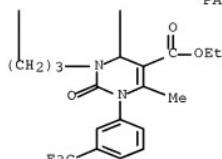
RN 904958-15-2 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-(biphenyl-2,2'-diyl bis(carbonyl-4,1-piperazinediyl-3,1-propanediyl))bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



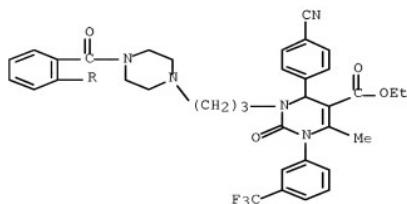
PAGE 2-A



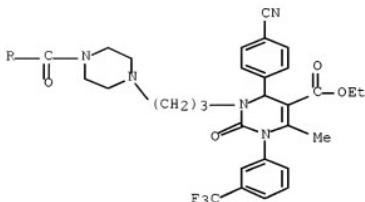
RN 904958-16-3 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-(1,2-phenylenebis(carbonyl-4,1-piperazinediyi-3,1-propanediyl)]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



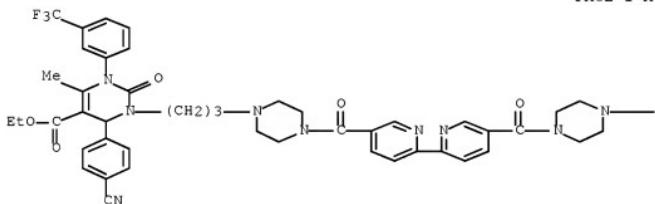
PAGE 2-A



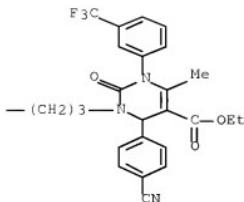
RN 904958-17-4 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-[{[2,2'-bipyridin]-5,5'-diyl}bis(carbonyl-4,1-piperazinediyl)-3,1-propanediyl]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



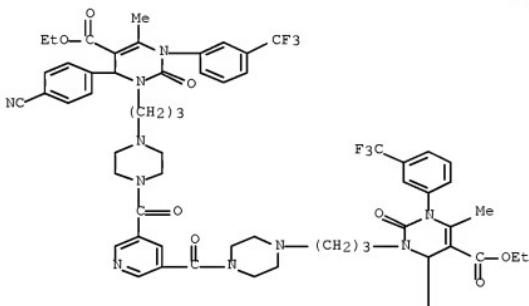
PAGE 1-B



RN 904958-18-5 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-(3,5-pyridinediyilbis(carbonyl-4,1-piperazinediyil-3,1-propanediyil))bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

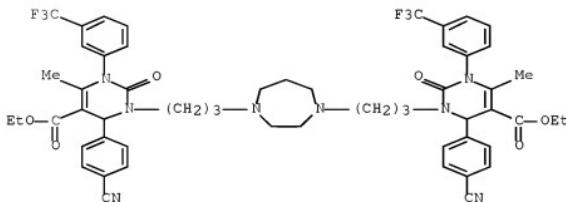


PAGE 2-A



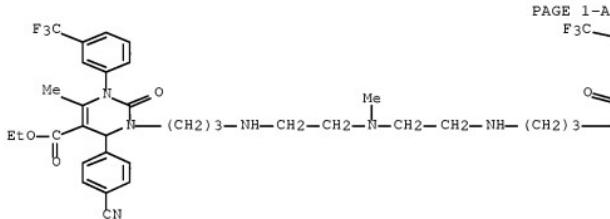
RN 904958-19-6 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-(tetrahydro-1H-1,4-diazepine-1,4(5H)-diyl)di-3,1-propanediyl]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)



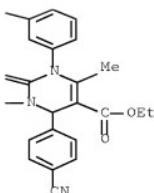
RN 904958-20-9 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-(methylimino)bis(2,1-ethanediylimino-3,1-propanediyl)]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)



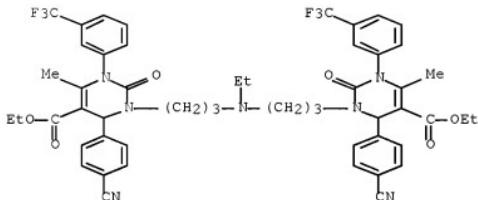
PAGE 1-A

PAGE 1-B



RN 904958-21-0 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-(ethylimino)di-2,1-ethanediyl]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)

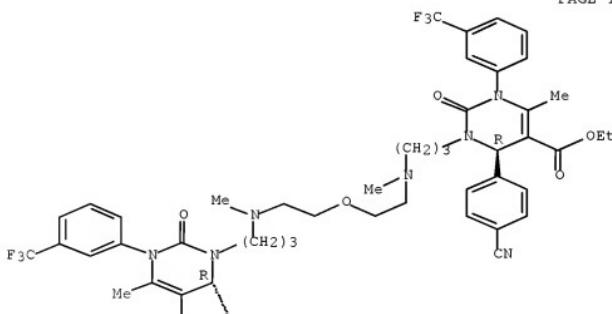


RN 904958-22-1 HCAPLUS

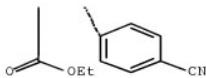
CN 5-Pyrimidinecarboxylic acid, 1,1'-(oxybis[2,1-ethanediyl(methylimino)-3,1-propanediyl])bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester, (6R,6'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A

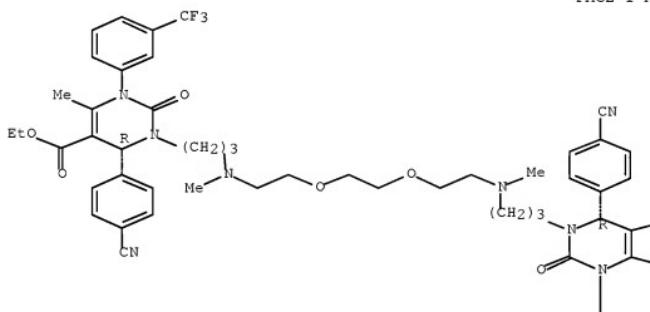


RN 904958-23-2 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-(4,13-dimethyl-7,10-dioxa-4,13-diazahexadecane-1,16-diyl)bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester, (6R,6'R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

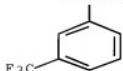


PAGE 1-B



—Me

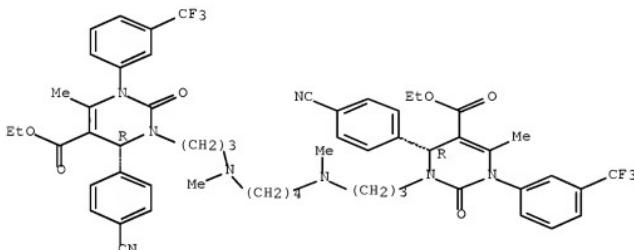
PAGE 2-A



RN 904958-24-3 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-[1,4-butanediylbis[(methylimino)-3,1-propanediyll]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)

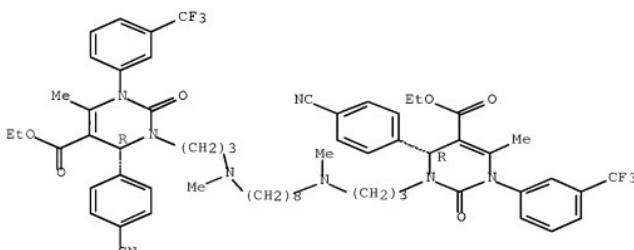
Absolute stereochemistry.



RN 904958-25-4 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-[1,8-octanediyllbis[(methylimino)-3,1-propanediyll]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)

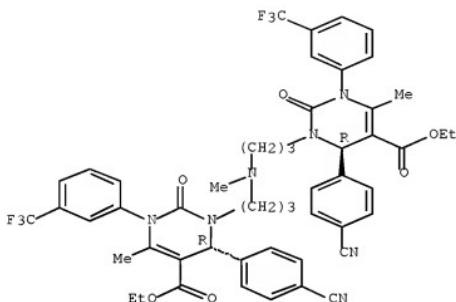
Absolute stereochemistry.



RN 904958-26-5 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-(methylimino)di-2,1-ethanediyl]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester, (6R,6'R)- (CA INDEX NAME)

Absolute stereochemistry.

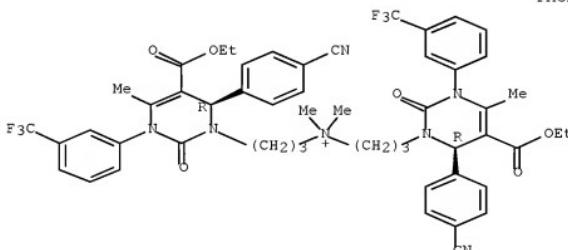


RN 904958-27-6 HCPLUS

CN 1(2H)-Pyrimidinopropanaminium, 6-(4-cyanophenyl)-N-[3-[(6R)-6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]propyl]-5-(ethoxycarbonyl)-3,6-dihydro-N,N,4-trimethyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, iodide (1:1), (6R)- (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

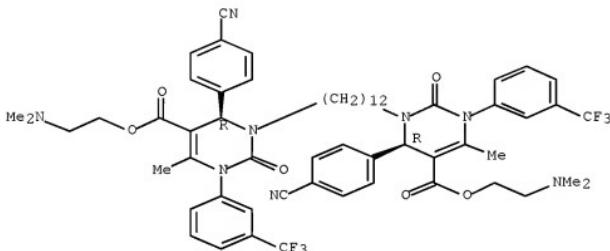


● I-

RN 904958-28-7 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-(1,12-dodecanediyl)bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, bis[2-(dimethylamino)ethyl] ester, (6R,6'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 904958-30-1 HCAPLUS

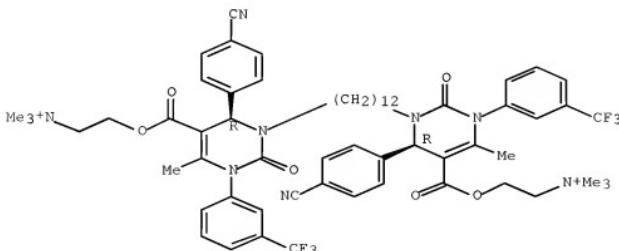
CN Ethanaminium, 2-{{((4R)-4-(4-cyanophenyl)-3-[12-[(6R)-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-5-[(2-(trimethylammonio)ethoxy]carbonyl]-1(2H)-pyrimidinyl)dodecyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-5-pyrimidinyl]carbonyloxy}-N,N,N-trimethyl-, formate (1:2) (CA INDEX NAME)

CM 1

CRN 904958-29-8

CMF C62 H74 F6 N8 O6

Absolute stereochemistry.



CM 2

CRN 71-47-6

CME C H O2

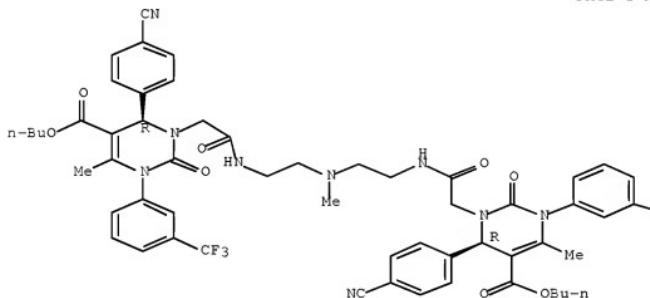


RN 904958-31-2 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 3-[2-[(2-[(2-[(2-[(6R)-5-(butoxycarbonyl)-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino)ethyl]methylamino]ethyl]amino]-2-oxoethyl]-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, butyl ester, (4R)- (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

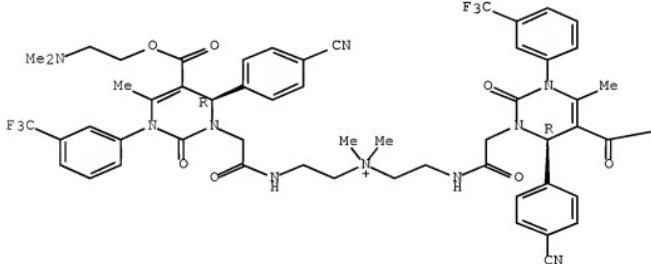


---CF_3

RN 904958-32-3 HCPLUS

CN Ethanaminium, 2-[(2-[(6R)-6-(4-cyanophenyl)-5-[(2-(dimethylamino)ethoxy]carbonyl]-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]-N-[2-[(2-[(6R)-6-(4-cyanophenyl)-5-[(2-(dimethylamino)ethoxy]carbonyl]-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl]-N,N-dimethyl-, iodide (1:1) (CA INDEX NAME)

Absolute stereochemistry.

 $\text{---O---CH}_2\text{CH}_2\text{NMe}_2$

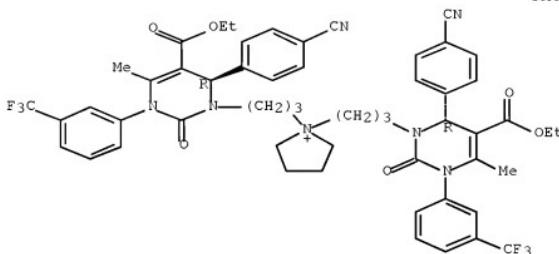
● I -

RN 904958-33-4 HCPLUS

CN Pyrrolidinium, 1,1-bis[3-[(6R)-6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]propyl]-, bromide (1:1) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A

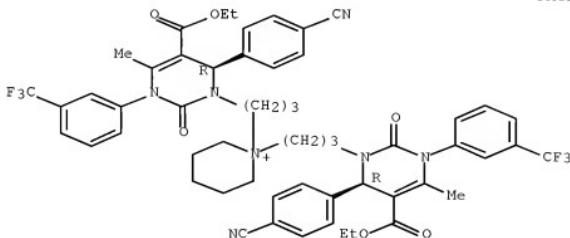
● Br -

RN 904958-34-5 HCPLUS

CN Piperidinium, 1,1-bis[3-[(6R)-6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]propyl]-, bromide (1:1) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



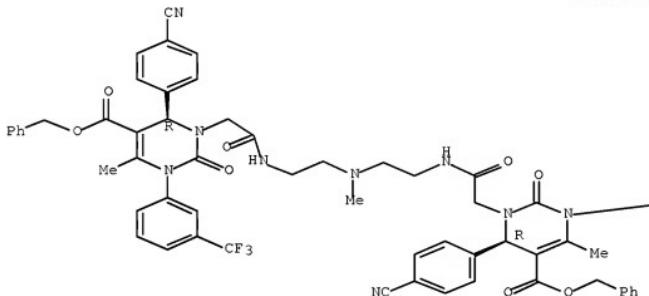
PAGE 2-A

● Br -

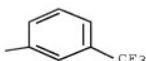
RN 904958-37-8 HCPLUS
 CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[[2-[(2-[(6R)-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-[(phenylmethoxy)carbonyl]-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl]methylamino]ethyl]amino]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, phenylmethyl ester, (4R)- (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



RN 904958-39-0 HCPLUS
 CN Ethanaminium, 2-[(2-[(6R)-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-

[(phenylmethoxy)carbonyl]-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino)-N-[2-[(2-[(6R)-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-[(phenylmethoxy)carbonyl]-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl]-N,N-dimethyl-, formate (1:1) (CA INDEX NAME)

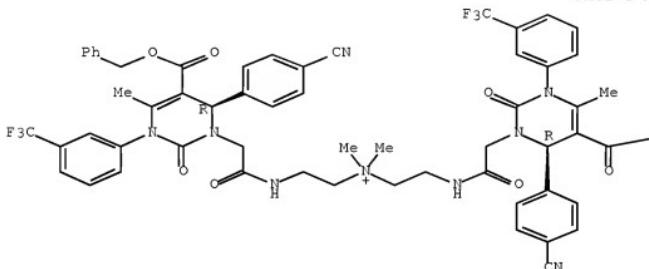
CM 1

CRN 904958-38-9

CMF C64 H58 F6 N9 O8

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



CM 2

CRN 71-47-6

CMF C H O2



RN 904958-41-4 HCAPLUS

CN Ethanaminium, 2-[(1(6R)-6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino-N-[2-[(1(6R)-6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl]-N,N-dimethyl-, butanedioate (2:1) (9CI) (CA INDEX NAME)

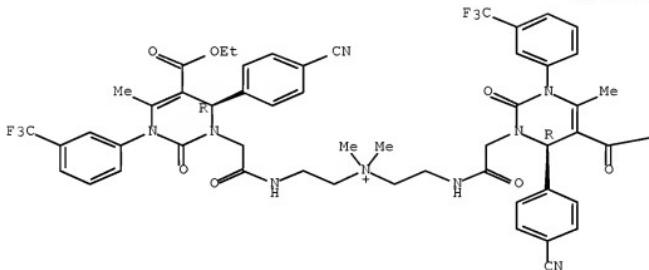
CM 1

CRN 904958-40-3

CMF C54 H54 F6 N9 O8

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

~~OEt~~

CM 2

CRN 56-14-4

CMF C4 H4 O4

-O₂C—CH₂—CH₂—CO₂-

IT 864228-16-0P 904958-45-8P

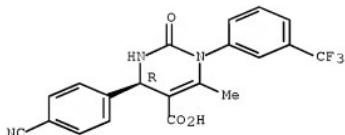
RL: PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (intermediate; preparation of multimers of tetrahydropyrimidinone compds.

as elastase inhibitors useful in the treatment of respiratory diseases)

RN 864228-16-0 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, (4R)- (CA INDEX NAME)

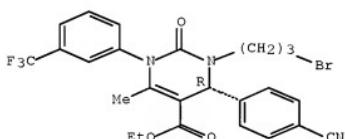
Absolute stereochemistry.



RN 904958-45-8 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 3-(3-bromopropyl)-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester, (4R)- (CA INDEX NAME)

Absolute stereochemistry.



IT 964151-33-7P 904958-42-5P 904958-43-6P

904958-44-7P 904958-46-9P 904958-47-0P

904958-48-1P 904958-49-2P 904958-50-5P

904958-51-6P 904958-52-7P 904958-53-8P

904958-54-9P 904958-55-0P 904958-56-1P

904958-57-2P 904958-58-3P 904958-59-4P

904958-60-7P 904958-61-6P 904958-62-9P

904958-63-0P 904958-64-1P 904958-65-2P

904958-66-3P 904958-67-4P 904958-68-5P

904958-69-6P 904958-70-9P 904958-71-0P

904958-72-1P 904958-73-2P 904958-74-3P

904958-75-4P 904958-76-5P 904958-77-6P

904958-78-7P 904958-79-8P 904958-80-1P

904958-31-2P 904958-83-4P 904958-97-0P
 904958-98-1P 904958-99-2P 904959-00-8P
 904959-01-9P 904959-02-0P 904959-03-1P
 904959-04-2P 904959-05-3P 904959-07-5P
 904959-08-6P 904959-16-6P 905287-66-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of multimers of tetrahydropyrimidinone compds.

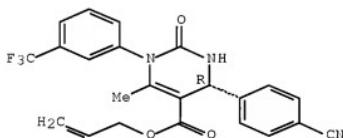
as

elastase inhibitors useful in the treatment of respiratory diseases)

RN 864151-33-7 HCPLUS

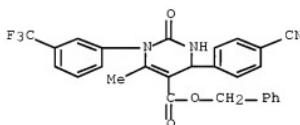
CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-propen-1-yl ester, (4R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 904958-42-5 HCPLUS

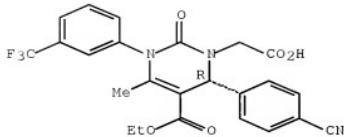
CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, phenylmethyl ester (CA INDEX NAME)



RN 904958-43-6 HCPLUS

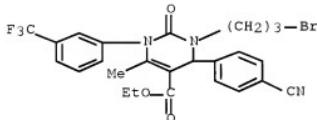
CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, (6R)- (CA INDEX NAME)

Absolute stereochemistry.



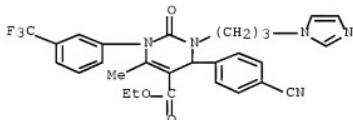
RN 904958-44-7 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 3-(3-bromopropyl)-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



RN 904958-46-9 HCPLUS

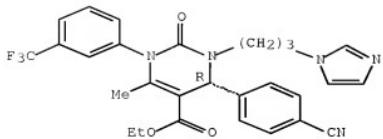
CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3-[3-(1H-imidazol-1-yl)propyl]-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



RN 904958-47-0 HCPLUS

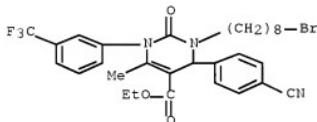
CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3-[3-(1H-imidazol-1-yl)propyl]-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester, (4R)- (CA INDEX NAME)

Absolute stereochemistry.



RN 904958-48-1 HCAPLUS

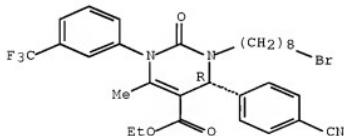
CN 5-Pyrimidinecarboxylic acid, 3-(8-bromoethyl)-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



RN 904958-49-2 HCAPLUS

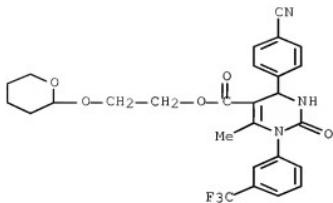
CN 5-Pyrimidinecarboxylic acid, 3-(8-bromoethyl)-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester, (4R)- (CA INDEX NAME)

Absolute stereochemistry.



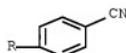
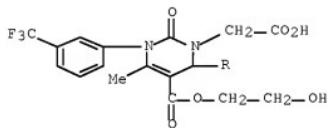
RN 904958-50-5 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-[(tetrahydro-2H-pyran-2-yl)oxy]ethyl ester (CA INDEX NAME)



RN 904958-51-6 HCPLUS

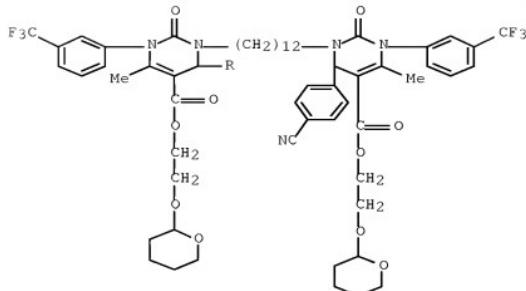
CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-5-[(2-hydroxyethoxy)carbonyl]-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



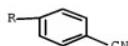
RN 904958-52-7 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-(1,12-dodecanediyl)bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-bis[2-[(tetrahydro-2H-pyran-2-yl)oxy]ethyl] ester (9CI) (CA INDEX NAME)

PAGE 1-A

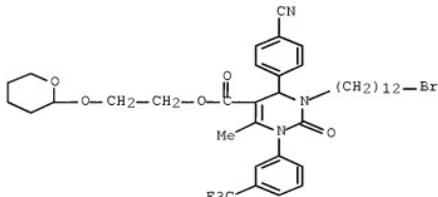


PAGE 2-A



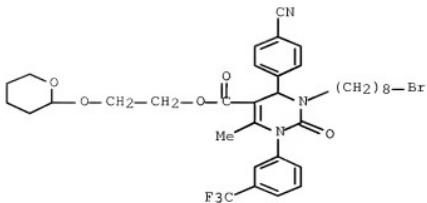
RN 904958-53-8 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 3-(12-bromododecyl)-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-[(tetrahydro-2H-pyran-2-yl)oxy]ethyl ester (CA INDEX NAME)



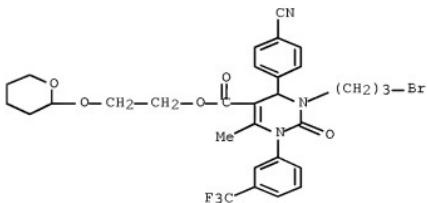
RN 904958-54-9 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 3-(8-bromo-13-cyano-octyl)-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-[(tetrahydro-2H-pyran-2-yl)oxy]ethyl ester (CA INDEX NAME)



RN 904958-55-0 HCPLUS

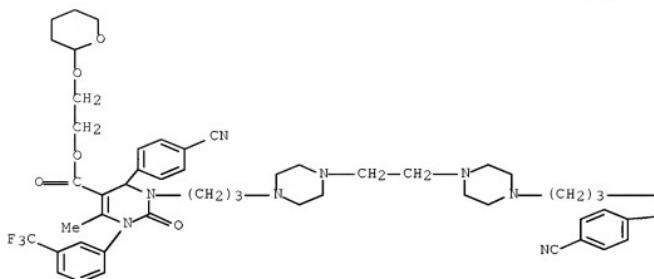
CN 5-Pyrimidinecarboxylic acid, 3-(3-bromopropyl)-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-[1(tetrahydro-2H-pyran-2-yl)oxy]ethyl ester (CA INDEX NAME)



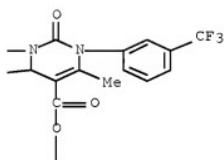
RN 904958-56-1 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-[1,2-ethanediylbis(4,1-piperazinediyl-3,1-propanediyl)]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, bis[2-[1(tetrahydro-2H-pyran-2-yl)oxy]ethyl] ester (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B

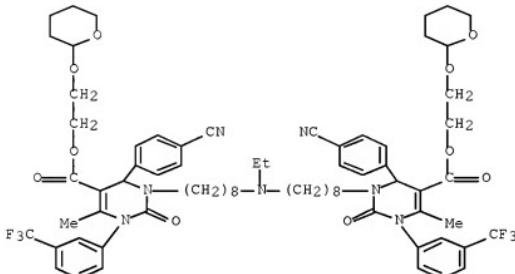


PAGE 2-B



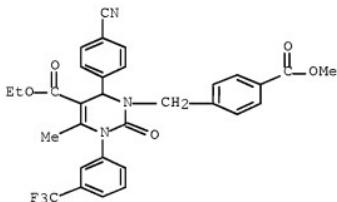
RN 904958-57-2 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-(ethylimino)di-8,1-octanediyil]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, bis[2-[(tetrahydro-2H-pyran-2-yl)oxy]ethyl]ester (9CI) (CA INDEX NAME)



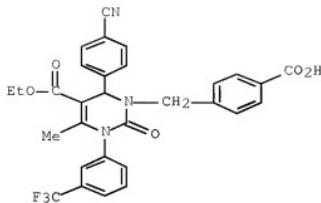
RN 904958-58-3 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3-[(4-(methoxycarbonyl)phenyl)methyl]-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



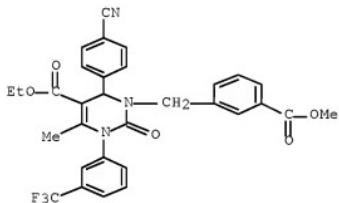
RN 904958-59-4 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 3-[(4-carboxyphenyl)methyl]-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 5-ethyl ester (CA INDEX NAME)



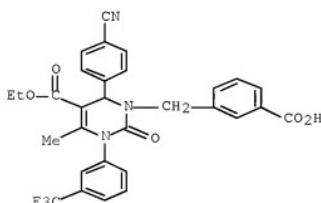
RN 904958-60-7 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3-[{3-(methoxycarbonyl)phenyl]methyl}-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



RN 904958-61-8 HCPLUS

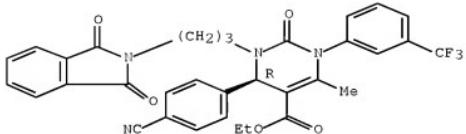
CN 5-Pyrimidinecarboxylic acid, 3-[{(3-carboxyphenyl)methyl}-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-(3-trifluoromethyl)phenyl]-, 5-ethyl ester (CA INDEX NAME)



RN 904958-62-9 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[3-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)propyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester, (4R)- (CA INDEX NAME)

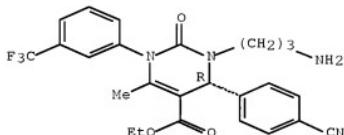
Absolute stereochemistry.



RN 904958-63-0 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 3-(3-aminopropyl)-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester, (4R)- (CA INDEX NAME)

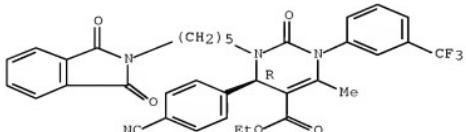
Absolute stereochemistry.



RN 904958-64-1 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[5-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)pentyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester, (4R)- (CA INDEX NAME)

Absolute stereochemistry.

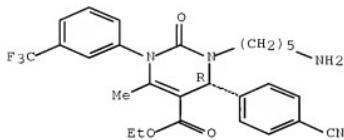


RN 904958-65-2 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 3-(5-aminopentyl)-4-(4-cyanophenyl)-1,2,3,4-

tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester,
 (4R)- (CA INDEX NAME)

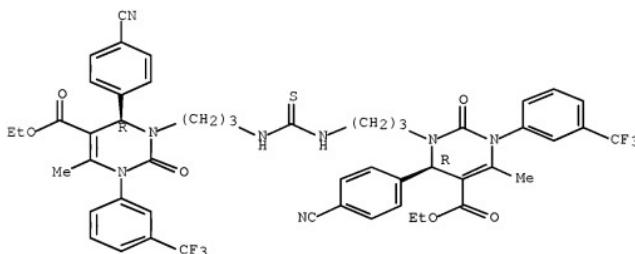
Absolute stereochemistry.



RN 904958-66-3 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-[carbonothioylbis(imino-3,1-propanediyl)]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester, (6R,6'R)- (9CI) (CA INDEX NAME)

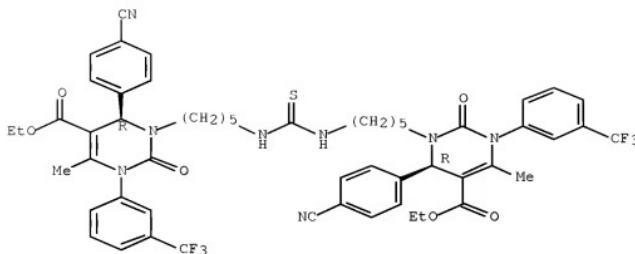
Absolute stereochemistry.



RN 904958-67-4 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-[carbonothioylbis(imino-5,1-pantanediyl)]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester, (6R,6'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

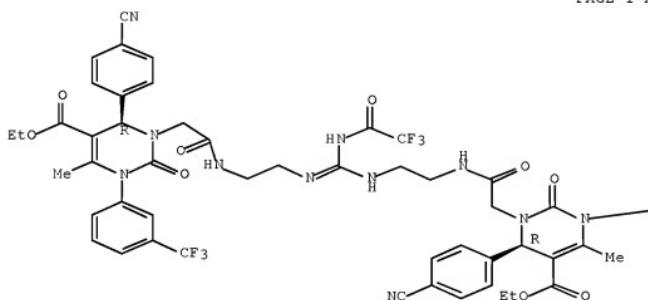


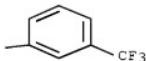
RN 904958-68-5 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-[2,12-dioxo-7-[(trifluoroacetyl)amino]-3,6,8,11-tetraaza-6-tridecene-1,13-diyl]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester, (6R,6'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

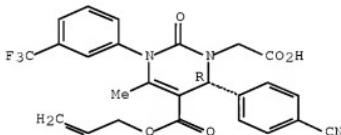




RN 904958-69-6 HCPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-[2-propen-1-yloxy]carbonyl-3-[3-(trifluoromethyl)phenyl]-, (6R)- (CA INDEX NAME)

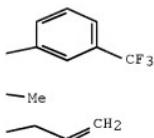
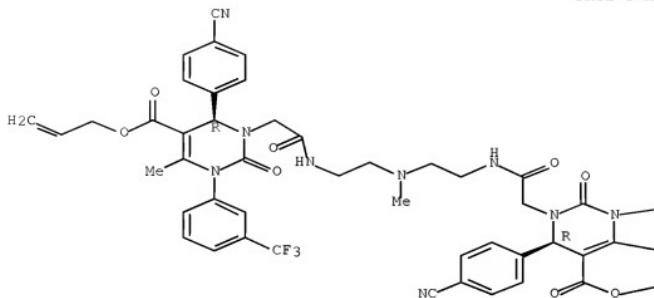
Absolute stereochemistry.



RN 904958-70-9 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[(2-[(2-[(6R)-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-[2-propen-1-yloxy]carbonyl)-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl]methylamino]ethyl]amino]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-propen-1-yl ester, (4R)- (CA INDEX NAME)

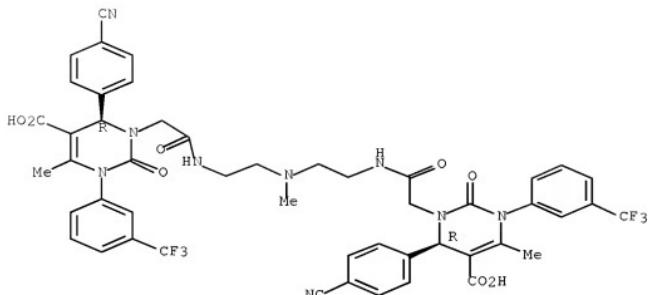
Absolute stereochemistry.



RN 904958-71-0 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 3-[2-[[2-[[2-[(6R)-5-carboxy-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinylacetylaminolethyl]methylaminolethyl]amino]-2-oxoethyl]-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, (4R)- (CA INDEX NAME)

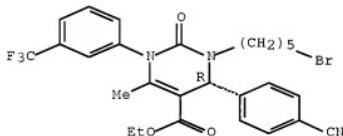
Absolute stereochemistry.



RN 904958-72-1 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 3-(5-bromopentyl)-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester, (4R)- (CA INDEX NAME)

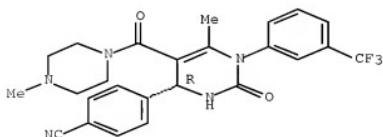
Absolute stereochemistry.



RN 904958-73-2 HCPLUS

CN Benzonitrile, 4-[(4R)-1,2,3,4-tetrahydro-6-methyl-5-[(4-methyl-1-piperazinyl)carbonyl]-2-oxo-1-[3-(trifluoromethyl)phenyl]-4-pyrimidinyl]- (CA INDEX NAME)

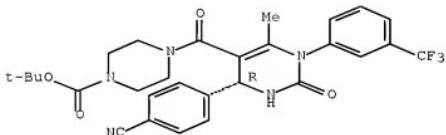
Absolute stereochemistry.



RN 904958-74-3 HCPLUS

CN 1-Piperazinecarboxylic acid, 4-[(4R)-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-5-pyrimidinyl]carbonyl-, 1,1-dimethylethyl ester (CA INDEX NAME)

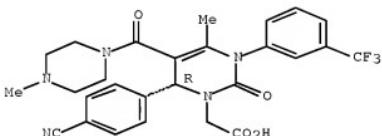
Absolute stereochemistry.



RN 904958-75-4 HCPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-5-[(4-methyl-1-piperazinyl)carbonyl]-2-oxo-3-[3-(trifluoromethyl)phenyl]-, (6R)- (CA INDEX NAME)

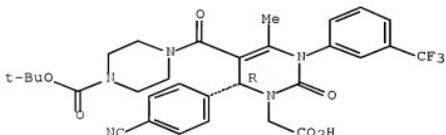
Absolute stereochemistry.



RN 904958-76-5 HCPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-[(4-[(1,1-dimethylethoxy)carbonyl]-1-piperazinyl)carbonyl]-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, (6R)- (CA INDEX NAME)

Absolute stereochemistry.



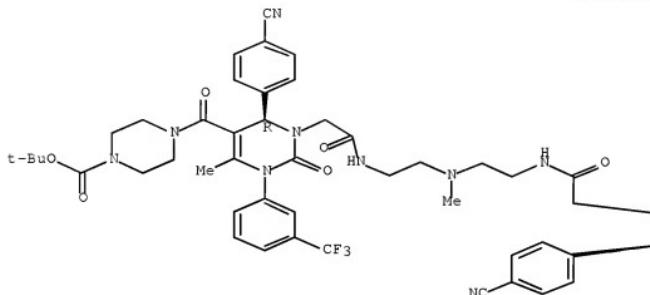
RN 904958-77-6 HCPLUS

CN 1-Piperazinecarboxylic acid, 4-[(4R)-4-(4-cyanophenyl)-3-[2-[2-[2-[2-

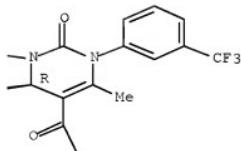
[(6R)-6-(4-cyanophenyl)-5-[[4-((1,1-dimethylethoxy)carbonyl)-1-piperazinyl]carbonyl]-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl)methylamino]ethylamino]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-5-pyrimidinyl]carbonyl]-, 1,1-dimethylethyl ester
(CA INDEX NAME)

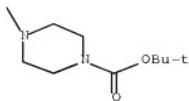
Absolute stereochemistry.

PAGE 1-A

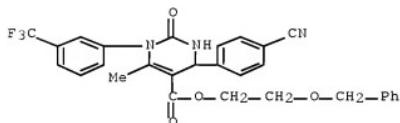


PAGE 1-B

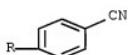
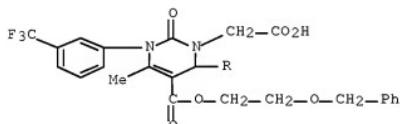




RN 904958-78-7 HCPLUS
 CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-(phenylmethoxy)ethyl ester (CA INDEX NAME)

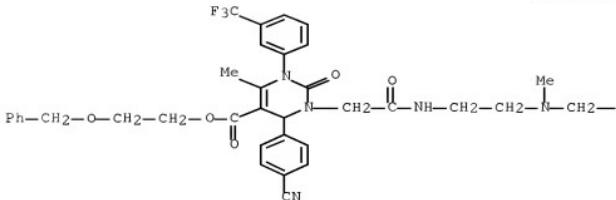


RN 904958-79-8 HCPLUS
 CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-[(2-(phenylmethoxy)ethoxy]carbonyl]-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

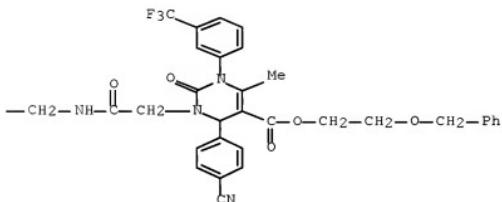


RN 904958-80-1 HCPLUS
 CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[[2-[[2-[[2-[(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-[(2-(phenylmethoxy)ethoxy]carbonyl]-3-[3-(trifluoromethyl)phenyl]1(2H)-pyrimidinyl]acetyl]amino]ethyl]methylamino]ethyl]amino]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-(phenylmethoxy)ethyl ester (CA INDEX NAME)

PAGE 1-A

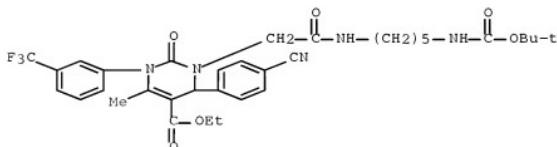


PAGE 1-B



RN 904958-81-2 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[{5-[{(1,1-dimethylethoxy)carbonyl]amino}pentyl]amino]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



RN 904958-83-4 HCPLUS

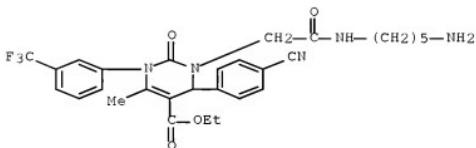
CN 5-Pyrimidinecarboxylic acid, 3-[2-[{(5-aminopentyl)amino}-2-oxoethyl]-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester, 2,2,2-trifluoroacetate (1:1) (CA

INDEX NAME)

CM 1

CRN 904958-82-3

CMF C29 H32 F3 N5 O4



CM 2

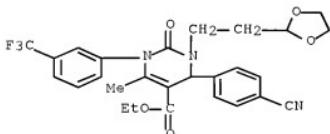
CRN 76-05-1

CMF C2 H F3 O2



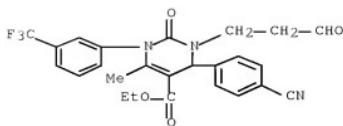
RN 904958-97-0 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-(1,3-dioxolan-2-yl)ethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-(3-(trifluoromethyl)phenyl)-, ethyl ester (CA INDEX NAME)



RN 904958-98-1 HCPLUS

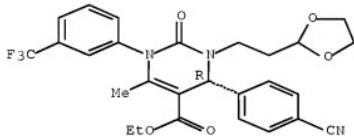
CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-3-(3-oxopropyl)-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



RN 904958-99-2 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-(1,3-dioxolan-2-yl)ethyl]-1,2,3,4-tetrahydro-6-methyl-1-[3-(trifluoromethyl)phenyl]-, ethyl ester, (4R)- (CA INDEX NAME)

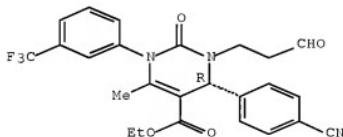
Absolute stereochemistry.



RN 904959-00-8 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-3-(3-oxopropyl)-1-[3-(trifluoromethyl)phenyl]-, ethyl ester, (4R)- (CA INDEX NAME)

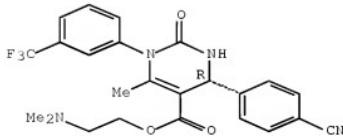
Absolute stereochemistry.



RN 904959-01-9 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-(dimethylamino)ethyl ester, (4R)- (CA INDEX NAME)

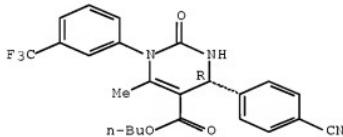
Absolute stereochemistry.



RN 904959-02-0 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, butyl ester, (4R)- (CA INDEX NAME)

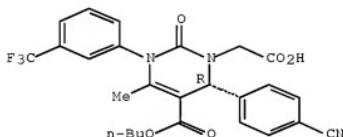
Absolute stereochemistry.



RN 904959-03-1 HCPLUS

CN 1(2H)-Pyrimidineacetic acid, 5-(butoxycarbonyl)-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, (6R)- (CA INDEX NAME)

Absolute stereochemistry.

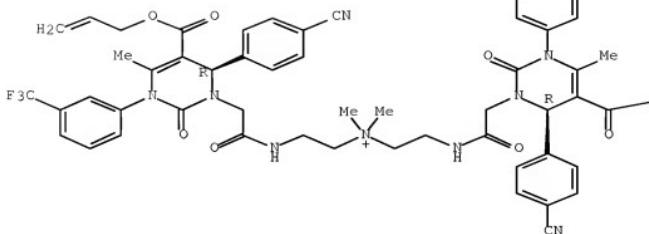


RN 904959-04-2 HCPLUS

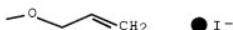
CN Ethanaminium, 2-[(2-[(6R)-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-[(2-propen-1-yloxy)carbonyl]-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]-N-[2-[(2-[(6R)-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-[(2-propen-1-yloxy)carbonyl]-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl]-N,N-dimethyl-, iodide (1:1) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

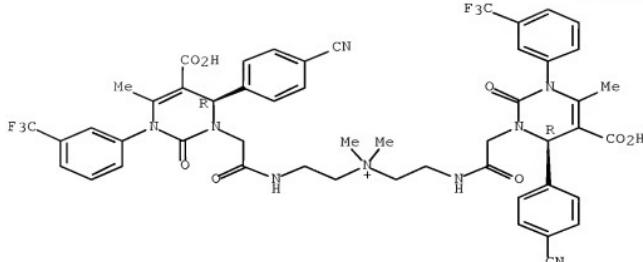


RN 904959-05-3 HCPLUS

CN Ethanaminium, 2-[{2-[(6R)-5-carboxy-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl}amino]-N-[2-[(2-[(6R)-5-carboxy-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl]-N,N-dimethyl-, iodide (1:1) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



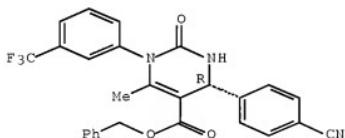
PAGE 2-A

● I-

RN 904959-07-5 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, phenylmethyl ester, (4R)- (CA INDEX NAME)

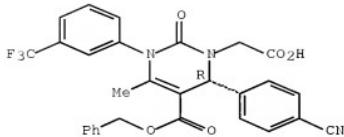
Absolute stereochemistry.



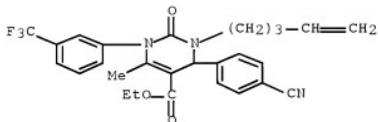
RN 904959-08-6 HCPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-[(phenylmethoxy)carbonyl]-3-[3-(trifluoromethyl)phenyl]-, (6R)- (CA INDEX NAME)

Absolute stereochemistry.

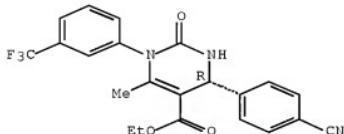


RN 904959-16-6 HCAPLUS
 CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-3-(4-penten-1-yl)-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)

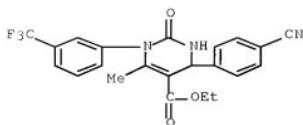


RN 905287-66-3 HCAPLUS
 CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester, (4R)- (CA INDEX NAME)

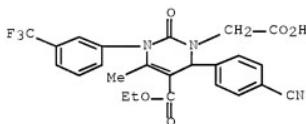
Absolute stereochemistry.



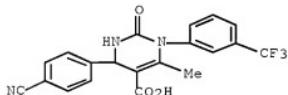
IT 671775-85-2 671776-27-5
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (starting material; preparation of multimers of tetrahydropyrimidinone compds. as elastase inhibitors useful in the treatment of respiratory diseases)
 RN 671775-85-2 HCAPLUS
 CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



RN 671776-27-5 HCPLUS
 CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

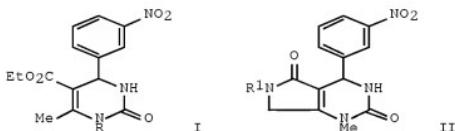


IT 671775-95-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (starting material; preparation of multimers of tetrahydropyrimidinone compds. as elastase inhibitors useful in the treatment of respiratory diseases)
 RN 671775-95-4 HCPLUS
 CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



L57 ANSWER 3 OF 15 HCPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 3
 ACCESSION NUMBER: 2001:779582 HCPLUS Full-text
 DOCUMENT NUMBER: 136:183781
 TITLE: Investigation of the chemical reactivity of positions N-3, C-5 and C6-methyl group in Biginelli type compounds and synthesis of new dihydropyrimidine derivatives
 AUTHOR(S): Namazi, H.; Mirzaei, Y. R.; Azamat, H.
 CORPORATE SOURCE: Lab of Carbohydrates and Biopolymers, Faculty of Chemistry, University of Tabriz, Tabriz, Iran
 SOURCE: Journal of Heterocyclic Chemistry (2001),

38(5), 1051-1054
 CODEN: JHTCAD; ISSN: 0022-152X
 PUBLISHER: HeteroCorporation
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 136:183781
 ED Entered STN: 26 Oct 2001
 GI



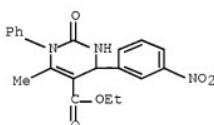
AB Biginelli-type compds. (I; R = Me, Ph) were prepared and converted to eight N-3 substituted dihydropyrimidines using NaH and various electrophiles (ClCO₂Et, TsCl, Ac₂O, AcCl and PhCOCl). I (R = Ph) was monobrominated at the C6-Me group using bromine solution. Reaction of the bromo derivative with amino nucleophiles, such as MeNH₂ and cyclohexylamine, produced two pyrrolopyrimidine derivs. (II; R₁ = Me, cyclohexyl). The structures of all the new compds. were confirmed using FTIR, ¹H NMR, and ¹³C NMR spectral and elemental analyses.

IT 321943-50-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (chemical reactivity of positions N-3, C-5 and C6-Me group in Biginelli type compds. and synthesis of new dihydropyrimidine derivs.)

RN 321943-50-4 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 1,2,3,4-tetrahydro-6-methyl-4-(3-nitrophenyl)-2-oxo-1-phenyl-, ethyl ester (CA INDEX NAME)

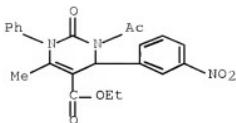


IT 398456-99-0P 398456-90-1P 398456-91-2P
 398456-96-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (chemical reactivity of positions N-3, C-5 and C6-Me group in Biginelli type compds. and synthesis of new dihydropyrimidine derivs.)

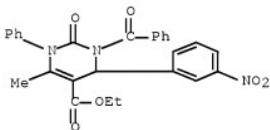
RN 398456-89-8 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 3-acetyl-1,2,3,4-tetrahydro-6-methyl-4-(3-nitrophenyl)-2-oxo-1-phenyl-, ethyl ester (CA INDEX NAME)



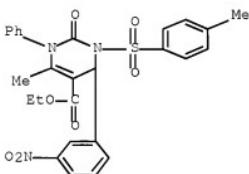
RN 398456-90-1 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 3-benzoyl-1,2,3,4-tetrahydro-6-methyl-4-(3-nitrophenyl)-2-oxo-1-phenyl-, ethyl ester (CA INDEX NAME)



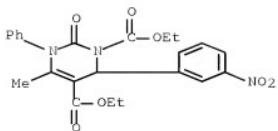
RN 398456-91-2 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 1,2,3,4-tetrahydro-6-methyl-3-[(4-methylphenyl)sulfonyl]-4-(3-nitrophenyl)-2-oxo-1-phenyl-, ethyl ester (CA INDEX NAME)



RN 398456-96-7 HCPLUS

CN 1,5(6H)-Pyrimidinedicarboxylic acid, 2,3-dihydro-4-methyl-6-(3-nitrophenyl)-2-oxo-3-phenyl-, diethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L57 ANSWER 4 OF 15 HCPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 4

ACCESSION NUMBER: 1997:1403324 HCPLUS Full-text

DOCUMENT NUMBER: 127:135777

TITLE: Diene-transmissive hetero-Diels-Alder reaction of cross-conjugated azatrienes: a novel and efficient method for the synthesis of ring-fused nitrogen heterocycles

AUTHOR(S): Saito, Takao; Kimura, Hiroaki; Chonan, Tomomichi; Soda, Takayuki; Karakasa, Takayuki

CORPORATE SOURCE: Dep. Chem., Faculty Sci., Sci. Univ. Tokyo, Tokyo, 162, Japan

SOURCE: Chemical Communications (Cambridge) (1997), (11), 1013-1014

CODEN: CHCOFS; ISSN: 1359-7345
PUBLISHER: Royal Society of Chemistry

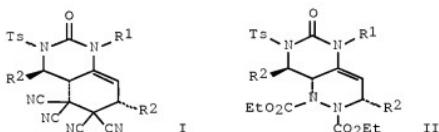
DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 127:135777

ED Entered STN: 30 Jun 1997

GI



AB A diene-transmissive hetero-Diels-Alder reaction of cross-conjugated azatrienes $R_2\text{CH}:\text{CH}(\text{C}(=\text{O})\text{NR}_1)\text{CH}:\text{CHR}_2$ ($R_1 = R_2 = \text{Ph}$; $R_1 = 4\text{-MeC}_6\text{H}_4\text{SO}_2$, $R_2 = \text{Ph}$; $R_1 = \text{PhCH}_2$, $R_2 = \text{Ph}$), which provides a novel and efficient synthetic method for ring-fused, nitrogen-heterocyclic frameworks such as quinazolin-2-ones, e.g., I, and pyrimido[5,4-c]pyridazin-6-ones, e.g., II, is described for the first time.

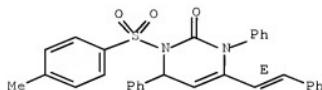
IT 192937-00-1P 192937-01-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(hetero-Diels-Alder of cross-conjugated azatrienes to give quinazolinones and pyrimidopyridazinones)

RN 192937-00-1 HCPLUS

CN 2(1H)-Pyrimidinone, 3,4-dihydro-3-[(4-methylphenyl)sulfonyl]-1,4-diphenyl-6-(2-phenylethenyl)-, (E)- (9CI) (CA INDEX NAME)

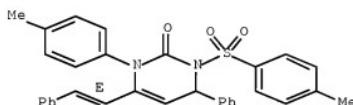
Double bond geometry as shown.



RN 192937-01-2 HCPLUS

CN 2(1H)-Pyrimidinone, 3,4-dihydro-1-(4-methylphenyl)-3-[(4-methylphenyl)sulfonyl]-4-phenyl-6-(2-phenylethenyl)-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L57 ANSWER 5 OF 15 HCPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 5

ACCESSION NUMBER: 1994:508678 HCPLUS [Full-text](#)

DOCUMENT NUMBER: 121:108678

TITLE: A simple approach to pyrimidine and quinazoline derivatives by [4+2] cycloaddition of 1,3-diazadienes and enamines

AUTHOR(S): Barluenga, Jose; Tomas, Miguel; Ballesteros, Alfredo; Lopez, Luis A.

CORPORATE SOURCE: Fac. Quim., Univ. Oviedo, Oviedo, 33071, Spain

SOURCE: Heterocycles (1994), 37(2), 1109-20

CODEN: HTCYAM; ISSN: 0385-5414

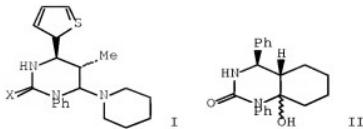
DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 121:108678

ED Entered STN: 03 Sep 1994

GI



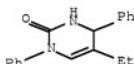
AB The reaction of 2-(trimethylsilyloxy)- and 2-(trimethylsilylthio)-1,3-diazabutadienes with enamines derived from aliphatic aldehydes leads regio- and stereoselectivity to substituted tetrahydropyrimidin-2(1H)-ones and thiones, e.g. I ($X = O, S$), in high yields. Extension of this cycloaddn. to cyclic enamines, e.g., derived from cyclohexanone, leading to quinazoline derivs., e.g. II, is also described. These heterocycles undergo hydrolysis and dehydration to 3,4-dihydropyrimidine and 3,4,5,6,7,8-hexahydroquinazoline derivs.

IT 126400-43-9P 156809-75-5P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

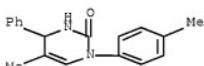
RN 126400-43-9 HCPLUS

CN 2(1H)-Pyrimidinone, 5-ethyl-3,4-dihydro-1,4-diphenyl- (CA INDEX NAME)



RN 156809-75-5 HCPLUS

CN 2(1H)-Pyrimidinone, 3,4-dihydro-5-methyl-1-(4-methylphenyl)-4-phenyl- (CA INDEX NAME)



L57 ANSWER 6 OF 15 HCPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 6

ACCESSION NUMBER: 1990:178861 HCPLUS Full-text

DOCUMENT NUMBER: 112:178861

ORIGINAL REFERENCE NO.: 112:30256h,30257a

TITLE: 1,4-Cycloaddition of 1,3-diazabutadienes with
enamines: an efficient route to the pyrimidine ring
Barluenga, Jose; Tomas, Miguel; Ballesteros, Alfredo;
Lopez, Luis A.

AUTHOR(S): Fac. Quim., Univ. Oviedo, Oviedo, 33071, Spain

CORPORATE SOURCE: Tetrahedron Letters (1989), 30(34), 4573-6
SOURCE:

DOCUMENT TYPE:

Journal

LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 112:178861

ED Entered STN: 12 May 1990

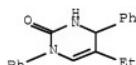
GI



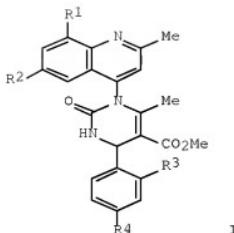
AB [4 + 2]Cycloaddn. reactions of 2-trimethylsilyloxy- and 2-trimethylsilylthio-1,3-diazabutadienes with enamines leading to pyrimidone derivs. are described. E.g., pyrimidine I was prepared from diazadiene II and (E)-1-pyrrolidino-1-butene.

IT 126400-43-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 126400-43-9 HCAPLUS
CN 2(1H)-Pyrimidinone, 5-ethyl-3,4-dihydro-1,4-diphenyl- (CA INDEX NAME)



L57 ANSWER 7 OF 15 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2002:199080 HCAPLUS Full-text
DOCUMENT NUMBER: 137:63219
TITLE: Arylquinolinylpyrimidones as antibacterial agents
AUTHOR(S): Machhi, Jigna; Patel, Dinesh; Desai, C. M.; Desai, Pratibha; Joshi, H. D.
CORPORATE SOURCE: Artemis Research Centre, Themis Chemical Ltd, Vapi,
396 185, India
SOURCE: Journal of the Institution of Chemists (India) (2001), 73(4), 140-142
PUBLISHER: Institution of Chemists (India)
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:63219
ED Entered STN: 19 Mar 2002
GI



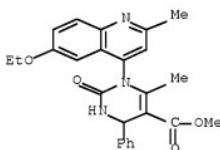
AB Title compds. I (R1 = Me, H; R2 = H, OMe, OEt; R3 = H, Cl, NO₂; R4 = H, OMe, NO₂) were synthesized and screened for their antibacterial activity.

IT 439079-03-5P 439079-05-7P 439079-06-8P
439079-10-4P 439079-11-5P 439079-12-6P
439079-13-7P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(arylquinolinylpyrimidones as antibacterial agents)

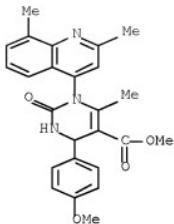
RN 439079-03-5 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 1-(6-ethoxy-2-methyl-4-quinoliny)-1,2,3,4-tetrahydro-6-methyl-2-oxo-4-phenyl-, methyl ester (CA INDEX NAME)



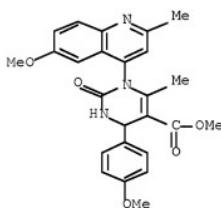
RN 439079-05-7 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 1-(2,8-dimethyl-4-quinoliny)-1,2,3,4-tetrahydro-4-(4-methoxyphenyl)-6-methyl-2-oxo-, methyl ester (CA INDEX NAME)



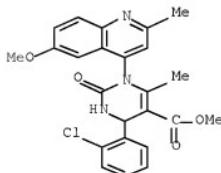
RN 439079-06-8 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 1,2,3,4-tetrahydro-1-(6-methoxy-2-methyl-4-quinolinyl)-4-(4-methoxyphenyl)-6-methyl-2-oxo-, methyl ester (CA INDEX NAME)



RN 439079-10-4 HCPLUS

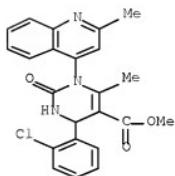
CN 5-Pyrimidinecarboxylic acid, 4-(2-chlorophenyl)-1,2,3,4-tetrahydro-1-(6-methoxy-2-methyl-4-quinolinyl)-6-methyl-2-oxo-, methyl ester (CA INDEX NAME)



RN 439079-11-5 HCPLUS

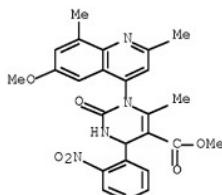
CN 5-Pyrimidinecarboxylic acid, 4-(2-chlorophenyl)-1,2,3,4-tetrahydro-6-

methyl-1-(2-methyl-4-quinolinyl)-2-oxo-, methyl ester (CA INDEX NAME)



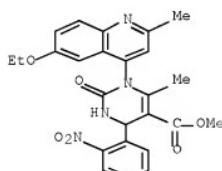
RN 439079-12-6 HCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,2,3,4-tetrahydro-1-(6-methoxy-2,8-dimethyl-4-quinolinyl)-6-methyl-4-(2-nitrophenyl)-2-oxo-, methyl ester (CA INDEX NAME)



RN 439079-13-7 HCAPLUS

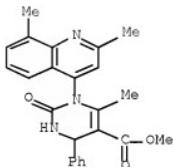
CN 5-Pyrimidinecarboxylic acid, 1-(6-ethoxy-2-methyl-4-quinolinyl)-1,2,3,4-tetrahydro-6-methyl-4-(2-nitrophenyl)-2-oxo-, methyl ester (CA INDEX NAME)

IT 439079-01-3P 439079-02-4P 439079-04-6P
439079-07-9P 439079-08-0P 439079-09-1P
439079-14-8P 439079-15-9P 439079-16-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (arylquinolinylpyrimidones as antibacterial agents)

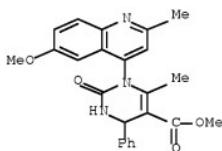
RN 439079-01-3 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 1-(2,8-dimethyl-4-quinolinyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-4-phenyl-, methyl ester (CA INDEX NAME)



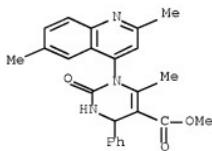
RN 439079-02-4 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 1,2,3,4-tetrahydro-1-(6-methoxy-2-methyl-4-quinolinyl)-6-methyl-2-oxo-4-phenyl-, methyl ester (CA INDEX NAME)



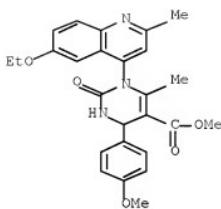
RN 439079-04-6 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 1-(2,6-dimethyl-4-quinolinyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-4-phenyl-, methyl ester (CA INDEX NAME)

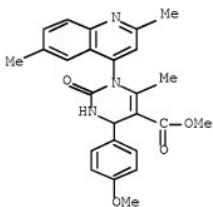


RN 439079-07-9 HCPLUS

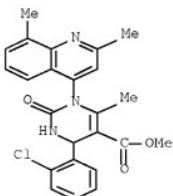
CN 5-Pyrimidinecarboxylic acid, 1-(6-ethoxy-2-methyl-4-quinolinyl)-1,2,3,4-tetrahydro-4-(4-methoxyphenyl)-6-methyl-2-oxo-, methyl ester (CA INDEX NAME)



RN 439079-08-0 HCPLUS
 CN 5-Pyrimidinecarboxylic acid, 1-(2,6-dimethyl-4-quinolinyl)-1,2,3,4-tetrahydro-4-(4-methoxyphenyl)-6-methyl-2-oxo-, methyl ester (CA INDEX NAME)

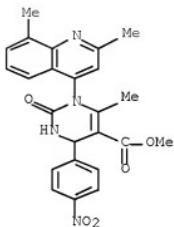


RN 439079-09-1 HCPLUS
 CN 5-Pyrimidinecarboxylic acid, 4-(2-chlorophenyl)-1-(2,6-dimethyl-4-quinolinyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-, methyl ester (CA INDEX NAME)



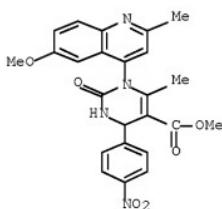
RN 439079-14-8 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 1-(2,8-dimethyl-4-quinolinyl)-1,2,3,4-tetrahydro-6-methyl-4-(4-nitrophenyl)-2-oxo-, methyl ester (CA INDEX NAME)



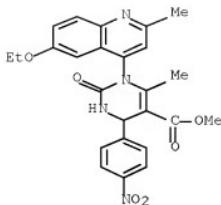
RN 439079-15-9 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 1,2,3,4-tetrahydro-1-(6-methoxy-2-methyl-4-quinolinyl)-6-methyl-4-(4-nitrophenyl)-2-oxo-, methyl ester (CA INDEX NAME)



RN 439079-16-0 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 1-(6-ethoxy-2-methyl-4-quinolinyl)-1,2,3,4-tetrahydro-6-methyl-4-(4-nitrophenyl)-2-oxo-, methyl ester (CA INDEX NAME)



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L57 ANSWER 8 OF 15 HCPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1998:795884 HCPLUS [Full-text](#)

DOCUMENT NUMBER: 130:125043

TITLE: A Combinatorial Approach to Recognition of Chirality:
Preparation of Highly Enantioselective

Aryl-Dihydropyrimidine Selectors for Chiral HPLC
Lewandowski, Kevin; Murer, Peter; Svec, Frantisek;
Frechet, Jean M. J.

AUTHOR(S): Department of Chemistry, University of California,
Berkeley, CA, 94720-1460, USA

CORPORATE SOURCE: Journal of Combinatorial Chemistry (1999),
1(1), 105-112

SOURCE: CODEN: JCCHFF; ISSN: 1520-4766
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal
LANGUAGE: English

ED Entered STN: 22 Dec 1998

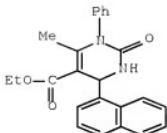
AB A parallel library of 108 4-aryl-1,4-dihydropyrimidine (DHPM) enantiomers, which are potential selectors for chiral HPLC sepn., was synthesized using the single-step Biginelli multicomponent condensation. The individual compds. were screened by observing the enantioselectivity for resolution on a brush-type L-(3,5-dinitrobenzoyl)leucine-based chiral stationary phase, and separation factors α up to 12 were achieved. The best candidates from the library contained an ortho-substituted aromatic group at C-4 of the pyrimidine ring and an alkyl substituent at N-1. Resolution of the enantiomers of the lead compound, 4-(9-phenanthryl)-1,4-dihydropyrimidine, using semipreparative chiral HPLC followed by attachment to monodisperse macroporous aminomethacrylate beads, provided a novel polymer based chiral stationary phase with good enantioselectivities in the resolution of several π -acidic arylidihydropyrimidines and derivatized profens. In addition, 3,5-dinitrobenzamido derivs. of α -amino acids could be resolved under normal phase HPLC conditions with separation factors up to 8.

IT 219814-96-7P 219814-97-8P

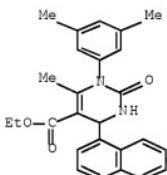
RL: PEP (Physical, engineering or chemical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(combinatorial synthesis and resolution of arylidihydropyrimidinecarboxylates for use as chiral stationary phases)

RN 219814-96-7 HCPLUS

CN 5-Pyrimidinecarboxylic acid, 1,2,3,4-tetrahydro-6-methyl-4-(1-naphthalenyl)-2-oxo-1-phenyl-, ethyl ester (CA INDEX NAME)



RN 219814-97-8 HCPLUS
 CN 5-Pyrimidinecarboxylic acid, 1-(3,5-dimethylphenyl)-1,2,3,4-tetrahydro-6-methyl-4-(1-naphthalenyl)-2-oxo-, ethyl ester (CA INDEX NAME)



REFERENCE COUNT: 69 THERE ARE 69 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L57 ANSWER 9 OF 15 HCPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1998:594082 HCPLUS Full-text
 DOCUMENT NUMBER: 129:269481
 TITLE: Synthesis and characterization of metal chelates with new pyrimidine derivatives
 AUTHOR(S): Siddiqi, K. S.; Nishat, N.
 CORPORATE SOURCE: Department of Chemistry, University of Bahrain, Isa Town, Bahrain
 SOURCE: Synthesis and Reactivity in Inorganic and Metal-Organic Chemistry (1998), 28(8), 1353-1369
 CODEN: SRIMCN; ISSN: 0094-5714
 PUBLISHER: Marcel Dekker, Inc.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 ED Entered STN: 18 Sep 1998
 AB The ligands 4-phenyl-5-ethoxycarbonyl-6-methyl-3,4-dihydropyrimidin-2-one (L1), 1,3-diacetamido(4-phenyl-5-ethoxycarbonyl-6-methyl-3,4-dihydropyrimidin-2-one) (L2) and 1,3-dipyrimidinyl(4-phenyl-5-ethoxycarbonyl-6-methyl-3,4-dihydropyrimidin-2-one) (L3) and their metal chelates with 3d metal ions were synthesized. The conductivity measurements suggest that [M(L1)2Cl2], [M2(L2)Cl4], [M'2(L2)Cl6] and [M(L3)2Cl2] are nonelectrolytes in DMSO and MeCN while [M'(L1)2Cl2]Cl and [M'(L3)2Cl2]Cl are 1:1 electrolytes, where M = Mn(II), Co(II), Ni(II), Cu(II) and Zn(II) and M' = Cr(III) and Fe(III). Spectroscopic studies show that L1 coordinates through NH and the O atom of the pyrimidinyl ring, L2 coordinates through the N and O atoms of the

amide group while L3 coordinates via the two N atoms of the pyrimidinone ring. The electronic spectra and the magnetic moments reveal that all metal complexes of L1, L3 and complexes of trivalent metal ions with L2 are octahedral while those of the divalent metal ions with L2 probably have a tetrahedral structure except for the Cu(II) complex which appears to be square-planar. The β values suggest a considerable degree of orbital overlap in the metal-ligand bond.

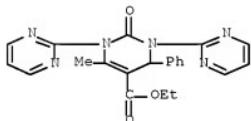
IT 213592-25-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and complexation with first-row transition-metal ions)

RN 213592-25-7 HCPLUS

CN [2,1'(2'H):3'(4'H),2''-Terpyrimidine]-5'-carboxylic acid,
4'-methyl-2'-oxo-6'-phenyl-, ethyl ester (9CI) (CA INDEX NAME)



IT 213592-48-4P 213592-50-8P 213592-52-0P

213592-54-2P 213592-56-4P 213592-58-6P

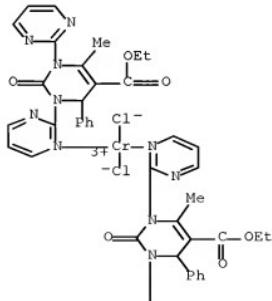
213592-60-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 213592-48-4 HCPLUS

CN Chromium(1+), dichlorobis[ethyl 6'-methyl-2'-oxo-4'-phenyl[2,1'(2'H):3'(4'H),2''-terpyrimidine]-5'-carboxylate- κ N1]-, chloride, (T-4)- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

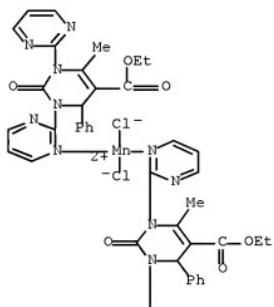


● Cl-

RN 213592-50-8 HCAPLUS

CN Manganese, dichlorobis[ethyl 6'-methyl-2'-oxo-4'-phenyl[2,1'(2'H):3'(4'H),2''-terpyrimidine]-5'-carboxylate-κNl]-
(9CI) (CA INDEX NAME)

PAGE 1-A



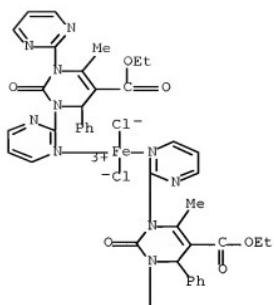
PAGE 2-A



RN 213592-52-0 HCAPLUS

CN Iron(II), dichlorobis[ethyl 6'-methyl-2'-oxo-4'-phenyl[2,1'(2'H):3'(4'H),2''-terpyrimidine]-5'-carboxylate-κNl]-chloride (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

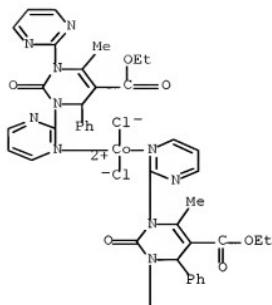


● Cl-

RN 213592-54-2 HCAPLUS

CN Cobalt, dichlorobis[ethyl 6'-methyl-2'-oxo-4'-phenyl[2,1'(2'H):3'(4'H),2'''-terpyrimidine]-5'-carboxylate-κN1]-, (T-4)- (9CI) (CA INDEX NAME)

PAGE 1-A



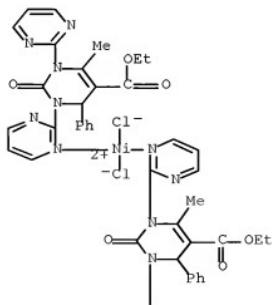
PAGE 2-A



RN 213592-56-4 HCPLUS

CN Nickel, dichlorobis[ethyl 6'-methyl-2'-oxo-4'-phenyl[2,1'(2'H):3'(4'H),2'''-terpyridine]-5'-carboxylate- $\kappa\text{N}1$]- (9CI) (CA INDEX NAME)

PAGE 1-A



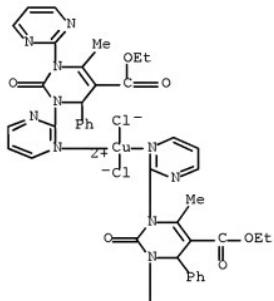
PAGE 2-A



RN 213592-58-6 HCPLUS

CN Copper, dichlorobis[ethyl 6'-methyl-2'-oxo-4'-phenyl[2,1'(2'H):3'(4'H),2''-terpyridine]-5'-carboxylate-κN1]- (9CI) (CA INDEX NAME)

PAGE 1-A



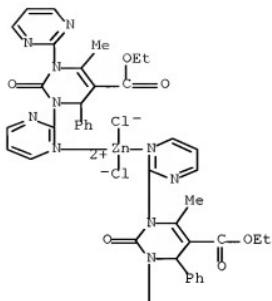
PAGE 2-A



RN 213592-60-0 HCPLUS

CN Zinc, dichlorobis[ethyl 6'-methyl-2'-oxo-4'-phenyl[2,1'(2'H):3'(4'H),2''-terpyridine]-5'-carboxylate-κN1]-, (T-4)- (9CI) (CA INDEX NAME)

PAGE 1-A

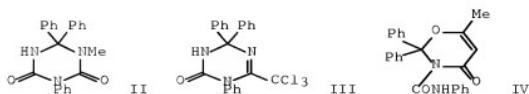


PAGE 2-A



REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L57 ANSWER 10 OF 15 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1976:592595 HCAPLUS Full-text
 DOCUMENT NUMBER: 85:192595
 ORIGINAL REFERENCE NO.: 85:30799a,30802a
 TITLE: Formation of heterocyclic compounds by use of
 N'-diphenylmethylen-N-phenyl-N-trimethylsilylurea
 AUTHOR(S): Matsuda, Isamu; Yamamoto, Sakae; Ishii, Yoshio
 CORPORATE SOURCE: Fac. Eng., Nagoya Univ., Nagoya, Japan
 SOURCE: Journal of the Chemical Society, Perkin Transactions
 1: Organic and Bio-Organic Chemistry (1972-1999) (1976), (14), 1523-8
 CODEN: JCPRB4; ISSN: 0300-922X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 ED Entered STN: 12 May 1984
 GI



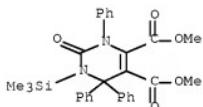
AB The reactions of the title urea (I) with acceptor mols. were studied. With cyclohexyl isocyanide, MeNCO, MeO2CC.tpbond.CCO2Me, or Cl3CCN followed by desilylation I underwent [4+1] or [4+2] cycloaddn.; imidazolidinone, triazinone, and pyrimidinone derivs. were formed. E.g., I with MeNCO gave the triazinone II. I reacted with RCN (R = CCl₃, NMe₂) to give the triazinone III and Ph₂C:NC(NMe₂):NPh, resp., by decomposition of the intermediate silyloxytriphenyltriazine with MeOH or under the reaction conditions, resp. Reaction of I with RR'CO (RR' = Ph₂C; R = H, R' = CCl₃) gave the insertion products Ph₂C:NCONPhCRR'OSiMe₃. Diketene reacted with I to give the oxazinone IV.

IT 61032-91-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and desilylation of)

RN 61032-91-5 HCPLUS

CN 4,5-Pyrimidinedicarboxylic acid, 1,2,3,6-tetrahydro-2-oxo-3,6,6-triphenyl-1-(trimethylsilyl)-, dimethyl ester (9CI) (CA INDEX NAME)

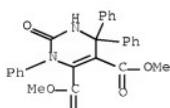


IT 61033-49-6F

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

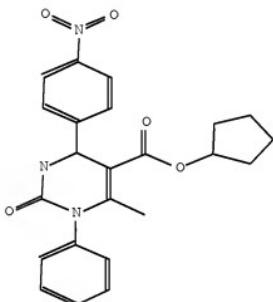
RN 61033-49-6 HCPLUS

CN 4,5-Pyrimidinedicarboxylic acid, 1,2,3,6-tetrahydro-2-oxo-3,6,6-triphenyl-, dimethyl ester (9CI) (CA INDEX NAME)



L57 ANSWER 11 OF 15 BEILSTEIN COPYRIGHT 2008 BEILSTEIN MDL on STN

Beilstein Records (BRN): 10596864
 Chemical Name (CN): 6-methyl-4-(4-nitro-phenyl)-2-oxo-1-phenyl-
 1,2,3,4-tetrahydro-pyrimidine-5-carboxylic
 acid cyclopentyl ester
 Autonom Name (AUN): 6-methyl-4-(4-nitro-phenyl)-2-oxo-1-phenyl-
 1,2,3,4-tetrahydro-pyrimidine-5-carboxylic
 acid cyclopentyl ester
 Molec. Formula (MF): C23 H23 N3 O5
 Molecular Weight (MW): 421.45
 Lawson Number (LN): 29411, 14131, 4999
 Compound Type (CTYPE): heterocyclic
 Constitution ID (CONSID): 8882785
 Tautomer ID (TAUTID): 9905640
 Entry Date (DED): 2007/04/15
 Update Date (DUPD): 2007/04/15



Field Availability:

| Code | Name | Occurrence |
|--------|-------------------|------------|
| BRN | Beilstein Records | 1 |
| CN | Chemical Name | 1 |
| AUN | Autonomname | 1 |
| MF | Molecular Formula | 1 |
| FW | Formular Weight | 1 |
| LN | Lawson Number | 3 |
| CTYPE | Compound Type | 1 |
| CONSID | Constitution ID | 1 |
| TAUTID | Tautomer ID | 1 |
| ED | Entry Date | 1 |
| UPD | Update Date | 1 |

This substance also occurs in Reaction Documents:

| Code | Name | Occurrence |
|-------|-------------------------------|------------|
| RX | Reaction Documents | 1 |
| RXPRO | Substance is Reaction Product | 1 |

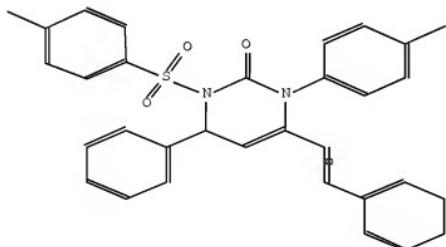
All References:

ALLREF

- Blackburn, Christopher; Guan, Bing; Brown, James; Cullis, Courtney; Condon, Stephen M.; Jenkins, Tracy J.; Peluso, Stephane; Ye, Yingchun; Gimeno, Ruth E.; Punreddy, Sandhya; Sun, Ying; et al., *Bioorg. Med. Chem. Lett.*, CODEN: BMCLE8, 16(13), <2006>, 3504 - 3509; BABS-6613616

L57 ANSWER 12 OF 15 BEILSTEIN COPYRIGHT 2008 BEILSTEIN MDL on STN

| | |
|---------------------------|---|
| Beilstein Records (BRN): | 7731869 |
| Chemical Name (CN): | 4-phenyl-6-styryl-3-(toluene-4-sulfonyl)-1-p-tolyl-3,4-dihydro-1H-pyrimidin-2-one |
| Autonom Name (AUN): | 4-phenyl-6-styryl-3-(toluene-4-sulfonyl)-1-p-tolyl-3,4-dihydro-1H-pyrimidin-2-one |
| Molec. Formula (MF): | C32 H28 N2 O3 S |
| Molecular Weight (MW): | 520.64 |
| Lawson Number (LN): | 28747, 14141, 13813 |
| File Segment (FS): | Stereo compound |
| Compound Type (CTYPE): | heterocyclic |
| Constitution ID (CONSID): | 6625170 |
| Tautomer ID (TAUTID): | 7353999 |
| Beilstein Citation (BSO): | 6-24 |
| Entry Date (DED): | 1997/11/18 |
| Update Date (DUPD): | 1998/03/04 |



Field Availability:

| Code | Name | Occurrence |
|--------|--------------------|------------|
| BRN | Beilstein Records | 1 |
| CN | Chemical Name | 1 |
| AUN | Autonomname | 1 |
| MF | Molecular Formula | 1 |
| FW | Formular Weight | 1 |
| LN | Lawson Number | 3 |
| FS | File Segment | 1 |
| CTYPE | Compound Type | 1 |
| CONSID | Constitution ID | 1 |
| TAUTID | Tautomer ID | 1 |
| BSO | Beilstein Citation | 1 |
| ED | Entry Date | 1 |
| UPD | Update Date | 1 |

This substance also occurs in Reaction Documents:

| Code | Name | Occurrence |
|-------|--------------------------------|------------|
| RX | Reaction Documents | 5 |
| RXREA | Substance is Reaction Reactant | 4 |
| RXPRO | Substance is Reaction Product | 1 |

All References:

ALLREF

- Saito, Takao; Kimura, Hiroaki; Chonan, Tomomichi; Soda, Takayuki; Karakasa, Takayuki, Chem.Commun., CODEN: CHCOFS(11), <1997>, 1013-1014; BABS-6058956

L57 ANSWER 13 OF 15 BEILSTEIN COPYRIGHT 2008 BEILSTEIN MDL on STN

| | |
|---------------------------|--|
| Beilstein Records (BRN): | 948115 |
| Beilstein Pref. RN (BPR): | 61033-49-6 |
| CAS Reg. No. (RN): | 61033-49-6 |
| Chemical Name (CN): | 2-oxo-3,6,6-triphenyl-1,2,3,6-tetrahydro-pyrimidine-4,5-dicarboxylic acid dimethyl ester |
| Autonom Name (AUN): | 2-oxo-3,6,6-triphenyl-1,2,3,6-tetrahydro-pyrimidine-4,5-dicarboxylic acid dimethyl ester |
| Molec. Formula (MF): | C26 H22 N2 O5 |
| Molecular Weight (MW): | 442.47 |
| Lawson Number (LN): | 29471, 14131, 289 |
| Compound Type (CTYPE): | heterocyclic |
| Constitution ID (CONSID): | 928678 |
| Tautomer ID (TAUTID): | 924038 |
| Beilstein Citation (BSO): | 5-25-08-00455 |
| Entry Date (DED): | 1988/11/28 |
| Update Date (DUPD): | 1993/11/10 |

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Field Availability:

| Code | Name | Occurrence |
|--------|----------------------------|------------|
| BRN | Beilstein Records | 1 |
| BPR | Beilstein Preferred RN | 1 |
| RN | CAS Registry Number | 1 |
| CN | Chemical Name | 1 |
| AUN | Autononname | 1 |
| MF | Molecular Formula | 1 |
| FW | Formular Weight | 1 |
| LN | Lawson Number | 3 |
| FS | File Segment | 1 |
| CTYPE | Compound Type | 1 |
| CONSID | Constitution ID | 1 |
| TAUTID | Tautomer ID | 1 |
| BSO | Beilstein Citation | 1 |
| ED | Entry Date | 1 |
| UPD | Update Date | 1 |
| IR | Infrared Spectrum | 1 |
| MP | Melting Point | 1 |
| MS | Mass Spectrum | 1 |
| NMR | Nuclear Magnetic Resonance | 1 |

This substance also occurs in Reaction Documents:

| Code | Name | Occurrence |
|-------|-------------------------------|------------|
| RX | Reaction Documents | 1 |
| RXPRO | Substance is Reaction Product | 1 |

All References:

ALLREF

1. Matsuda,I. et al., J.Chem.Soc.Perkin Trans.1, CODEN: JCPRB4, <1976>, 1523-1528

- L57 ANSWER 14 OF 15 BABS COPYRIGHT 2008 BEILSTEIN MDL on STN
AN 6679519 BABS Full-text
- TI N-Substituted Ureas and Thioureas in Biginelli Reaction Promoted by Chlorotrimethylsilane: Convenient Synthesis of N1-Alkyl-, N1-Aryl-, and N1,N3-Dialkyl-3,4-Dihydropyrimidin-2(1H)-(thi)ones
- AU Ryabukhin, Sergey V.; Plaskon, Andrey S.; Ostapchuk, Eugeniy N.; Volochnyuk, Dmitriy M.; Tolmachov, Andrey A.
- SO Synthesis (2007), (3), 417 - 427
- CODEN: SYNTBF
- DT Journal
- AB The classical Biginelli reaction has been extended by the use of N-substituted ureas and thioureas. A set of N1-alkyl-, N1-aryl-, and N1,N3-dialkyl-3,4-dihydropyrimidin-2(1H)-(thi)ones was readily prepared in excellent yield when chlorotrimethylsilane in N,N-dimethylformamide was used as promoter and water scavenger.
- CT Biginelli reaction; heterocycles; Lewis acid; multicomponent reaction; parallel synthesis
- L57 ANSWER 15 OF 15 BABS COPYRIGHT 2008 BEILSTEIN MDL on STN
AN 6615225 BABS Full-text
- TI A Convenient Synthesis of N1-Substituted 3,4-Dihydropyrimidin-2(1H)-ones

by Cyclocondensation of α -Chlorobenzyl Isocyanates with Ethyl N-alkyl(aryl)- β -aminocrotonates

AU Sukach, Volodymyr A.; Bol'but, Andriy V.; Sinitsa, Anatoliy D.; Vovk, Mykhaylo V.

SO Syn. Lett. (2006), (3), 375 - 378

CODEN: SYNLES

DT Journal

AB A new convenient approach to the synthesis of N1-substituted 3,4-dihydropyrimidin-2(1H)-ones was developed using the regioselective cyclocondensation of α -chlorobenzyl isocyanates with ethyl N-alkyl(aryl)- β -aminocrotonates. A number of N1-aryl and N1-alkyl substituted Biginelli compounds difficult to obtain by other methods were prepared with high yields.

CT cyclocondensation; regioselectivity; α -chloroalkyl isocyanates;

dihydropyrimidones; β -aminocrotonic esters

Search History

L1 1 SEA ABB=ON PLU=ON US2007-590786/APPS

FILE 'REGISTRY' ENTERED AT 11:04:13 ON 15 APR 2008
L2 157 SEA ABB=ON PLU=ON (10130-89-9/B1 OR 105-07-7/B1 OR 106-95-6/B
I OR 108052-76-2/B1 OR 1118-84-9/B1 OR 1129-28-8/B1 OR
123-54-6/B1 OR 126062-63-3/B1 OR 13114-87-9/B1 OR 131747-68-7/B
I OR 13831-03-3/B1 OR 140-88-5/B1 OR 141-97-9/B1 OR 157312-16-8
/B1 OR 1620-77-5/B1 OR 177278-22-7/B1 OR 208465-72-9/B1 OR
2144-37-8/B1 OR 220510-74-7/B1 OR 26690-80-2/B1 OR 30379-58-9/B
I OR 3119-02-6/B1 OR 3510-66-5/B1 OR 3587-60-8/B1 OR 4530-20-5/
BI OR 5292-43-3/B1 OR 540-51-2/B1 OR 5470-11-1/B1 OR 58553-48-3
/B1 OR 6165-68-0/B1 OR 6325-93-5/B1 OR 671775-85-2/B1 OR
671775-86-3/B1 OR 671775-93-2/B1 OR 671775-95-4/B1 OR 671776-48
-0/B1 OR 671776-50-4/B1 OR 671776-53-7/B1 OR 671776-55-9/B1 OR
67497-95-4/B1 OR 675103-35-2/B1 OR 675103-36-3/B1 OR 7307-03-1/
BI OR 7693-46-1/B1 OR 823-78-9/B1 OR 830-43-3/B1 OR 864150-42-5
/B1 OR 864150-44-7/B1 OR 864150-46-9/B1 OR 864150-48-1/B1 OR
864150-50-5/B1 OR 864150-52-7/B1 OR 864150-53-8/B1 OR 864150-54
-9/B1 OR 864150-55-0/B1 OR 864150-56-1/B1 OR 864150-57-2/B1 OR
864150-58-3/B1 OR 864150-59-4/B1 OR 864150-60-7/B1 OR 864150-61
-8/B1 OR 864150-62-9/B1 OR 864150-63-0/B1 OR 864150-64-1/B1 OR
864150-65-2/B1 OR 864150-66-3/B1 OR 864150-67-4/B1 OR 864150-68
-5/B1 OR 864150-69-6/B1 OR 864150-70-9/B1 OR 864150-71-0/B1 OR
864150-72-1/B1 OR 864150-73-2/B1 OR 864150-74-3/B1 OR 864150-75
-4/B1 OR 864150-76-5/B1 OR 864150-77-6/B1 OR 864150-78-7/B1 OR
864150-79-8/B1 OR 864150-80-1/B1 OR 864150-81-2/B1 OR 864150-82
-3/B1 OR 864150-83-4/B1 OR 864150-84-5/B1 OR 864150-85-6/B1 OR
864150-86-7/B1 OR 864150-87-8/B1 OR 864150-88-9/B1 OR 864150-89
-0/B1 OR 864150-90-3/B1 OR 864150-91-4/B1 OR 864150-92-5/B1 OR
864150-93-6/B1 OR 864150-94-7/B1 OR 864150-95-8/B1 OR 864150-96
-9/B1 OR 864150-97-0/B1 OR 864150-98-1/B1 OR 864150-99-2/B1 OR
864151-00-8/B1 OR 864151-01-9/B1 OR 864151-02-0/B1 OR 864151-0
L3 116 SEA ABB=ON PLU=ON L2 AND NR>=3
L4 116 SEA ABB=ON PLU=ON L3 AND NR>=2 AND O>=1
L5 STRUCTURE uploaded
L6 45 SEA SSS SAM L5
L7 10 SEA ABB=ON PLU=ON L2 AND L6
L8 741 SEA SSS FUL L5

FILE 'HCAPLUS' ENTERED AT 11:39:59 ON 15 APR 2008
L9 18 SEA ABB=ON PLU=ON L8

FILE 'REGISTRY' ENTERED AT 11:40:10 ON 15 APR 2008
L10 108 SEA ABB=ON PLU=ON L8 AND L2

FILE 'REGISTRY' ENTERED AT 11:44:22 ON 15 APR 2008
L11 STRUCTURE uploaded
L12 45 SEA SSS SAM L11
L13 STRUCTURE uploaded
L14 46 SEA SSS SAM L13
L15 767 SEA SSS FUL L13

FILE 'HCAPLUS' ENTERED AT 11:49:53 ON 15 APR 2008
L16 20 SEA ABB=ON PLU=ON L15

L17 17 SEA ABB=ON PLU=ON GIELEN-HAERTWIG H?/AU
 L18 233 SEA ABB=ON PLU=ON ALBRECHT? B?/AU
 L19 92 SEA ABB=ON PLU=ON KELDENICH J?/AU
 L20 843 SEA ABB=ON PLU=ON LI V?/AU
 L21 51 SEA ABB=ON PLU=ON PERNERSTORFER J?/AU
 L22 117 SEA ABB=ON PLU=ON SCHLEMMER K?/AU
 L23 22 SEA ABB=ON PLU=ON TELAN L?/AU
 L24 1299 SEA ABB=ON PLU=ON (L17 OR L18 OR L19 OR L20 OR L21 OR L22 OR
 L23)
 L25 6 SEA ABB=ON PLU=ON L24 AND L16
 L26 15 SEA ABB=ON PLU=ON L16 AND (PRY<=2005 OR AY<=2005 OR PY<=2005)
 L27 5 SEA ABB=ON PLU=ON L25 AND (PRY<=2005 OR AY<=2005 OR PY<=2005)

FILE 'WPIX' ENTERED AT 11:54:47 ON 15 APR 2008
 L28 13 SEA SSS SAM L13
 L29 117 SEA SSS FUL L13
 L30 7 SEA ABB=ON PLU=ON L29/DCR
 L31 6 SEA ABB=ON PLU=ON L30 AND (PRY<=2005 OR AY<=2005 OR PY<=2005)
 L32 4 SEA ABB=ON PLU=ON L31 AND L24

FILE 'BEILSTEIN' ENTERED AT 11:56:19 ON 15 APR 2008
 L33 1 SEA SSS SAM L13
 L34 23 SEA SSS FUL L13
 L35 20 SEA ABB=ON PLU=ON L34 AND BABSAN/FA
 SEL BABSAN

FILE 'BABS' ENTERED AT 11:57:00 ON 15 APR 2008
 L36 6 SEA ABB=ON PLU=ON (6615225/BABSAN OR 6322274/BABSAN OR
 6679519/BABSAN OR 5898555/BABSAN OR 5545785/BABSAN OR 6058956/B
 ABSAN)

FILE 'BEILSTEIN' ENTERED AT 11:57:38 ON 15 APR 2008
 L37 3 SEA ABB=ON PLU=ON L34 NOT L35

FILE 'REGISTRY' ENTERED AT 12:08:30 ON 15 APR 2008
 L38 STRUCTURE UPLOADED
 L39 46 SEA SSS SAM L38
 L40 768 SEA SSS FUL L38
 L41 108 SEA ABB=ON PLU=ON L40 AND L2

FILE 'HCAPLUS' ENTERED AT 12:11:54 ON 15 APR 2008
 L42 20 SEA ABB=ON PLU=ON L40
 L43 15 SEA ABB=ON PLU=ON L42 AND (PRY<=2005 OR AY<=2005 OR PY<=2005)
 L44 5 SEA ABB=ON PLU=ON L24 AND L43

FILE 'WPIX' ENTERED AT 12:13:15 ON 15 APR 2008
 L45 13 SEA SSS SAM L38
 L46 117 SEA SSS FUL L38
 L47 7 SEA ABB=ON PLU=ON L46/DCR
 L48 5 SEA ABB=ON PLU=ON L47 AND L24

FILE 'BEILSTEIN' ENTERED AT 12:14:49 ON 15 APR 2008
 L49 1 SEA SSS SAM L38
 L50 23 SEA SSS FUL L38
 L51 20 SEA ABB=ON PLU=ON L50 AND BABSAN/FA

FILE 'BABS' ENTERED AT 12:16:20 ON 15 APR 2008
 L52 6 SEA ABB=ON PLU=ON (6615225/BABSAN OR 6322274/BABSAN OR
 6679519/BABSAN OR 5898555/BABSAN OR 5545785/BABSAN OR 6058956/B

ABSAN)

L53 FILE 'BEILSTEIN' ENTERED AT 12:16:34 ON 15 APR 2008
3 SEA ABB=ON PLU=ON L50 NOT L51

L54 FILE 'HCAPLUS, WPIX' ENTERED AT 12:19:02 ON 15 APR 2008
6 DUP REM L44 L48 (4 DUPLICATES REMOVED)

L55 FILE 'HCAPLUS' ENTERED AT 12:19:55 ON 15 APR 2008
10 SEA ABB=ON PLU=ON L43 NOT L44

L56 FILE 'WPIX' ENTERED AT 12:20:16 ON 15 APR 2008
2 SEA ABB=ON PLU=ON L47 NOT L48

L57 FILE 'HCAPLUS, WPIX, BEILSTEIN, BABS' ENTERED AT 12:21:04 ON 15 APR 2008
15 DUP REM L55 L56 L53 L52 (6 DUPLICATES REMOVED)